Supporting Information

Structure and Excited-State Dynamics of Dimeric Copper(I) photosensitizers Investigated by Time-resolved X-ray and Optical Transient Absorption Spectroscopy

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Table of Contents	**Page No.**

Experimental Details

Extended X-ray Absorption Fine Structure (EXAFS) Analysis. Athena software[1, 2] was used for data processing. The energy scale for each scan was normalized using copper metal standard. Data in energy space were pre-edge corrected, normalized, deglitched (if necessary), and background corrected. The processed data were next converted to the photoelectron wave vector (k) space and weighted by k^2. The electron wave number is defined as $k = [2m(E - E_0)/\hbar^2]^{1/2}$, E_0 is the energy origin or the threshold energy. K-space data were truncated near the zero crossings k = 2 to 11.2 Å^{-1} for all **C1-C3** in Cu EXAFS Fourier transformation. The k-space data were transferred into the Artemis Software for curve fitting. In order to fit the data, the Fourier peaks were isolated separately, grouped together, or the entire (unfiltered) spectrum was used. The individual Fourier peaks were isolated by applying a Hanning window to the first and last 15% of the chosen range, leaving the middle 70% untouched. Curve fitting was performed using *ab initio*-calculated phases and amplitudes from the FEFF8[2] program from the University of Washington. *Ab initio*-calculated phases and amplitudes were used in the EXAFS equation (Equation 1),

$$\chi(k) = S_0^2 \sum_j \frac{N_j}{kR_j^2} f_{eff_j}(\pi, k, R_j) e^{-2\sigma_j^2 k^2} e^{\frac{-2R_j}{\lambda_j(k)}} \sin(2kR_j + \phi_{ij}(k)) \qquad \text{(Equation S1)}$$

where N_j is the number of atoms in the j^{th} shell; R_j the mean distance between the absorbing atom and the atoms in the j^{th} shell; $f_{eff_j}(\pi, k, R_j)$ is the *ab initio* amplitude function for shell *j*, and the Debye-Waller term $e^{-2\sigma_j^2 k^2}$ accounts for damping due to static and thermal disorder in absorber-backscatterer distances. The mean free path term $e^{\frac{-2R_j}{\lambda_j(k)}}$ reflects losses due to inelastic scattering, where $\lambda_j(k)$, is the electron mean free path. The oscillations in the EXAFS spectrum are reflected in the sinusoidal term $\sin(2kR_j + \phi_{ij}(k))$, where $\phi_{ij}(k)$ is the *ab initio* phase function for shell *j*. This sinusoidal term shows the direct relation between the frequency of the EXAFS oscillations in k-space and the absorber-backscatterer distance. S_0^2 is an amplitude reduction factor.

The EXAFS equation[3] (Eq. S1) was used to fit the experimental Fourier isolated data (q-space) as well as unfiltered data (k-space) and Fourier transformed data (R-space) using *N*, S_0^2, E_0, *R*, and σ^2 as variable parameters (Table S1). *N* refers to the number of coordination atoms surrounding Cu for each shell. The quality of fit was evaluated by R-factor and the reduced Chi^2 value. The deviation in E_0 ought to be less than or equal to 10 eV. R-factor less than 2% denotes that the fit is good enough. R-factor between 2 and 5% denotes that the fit is correct within a consistently broad model. The reduced Chi^2 value is used to compare fits as more absorber-backscatter shells are included to fit the data. A smaller reduced Chi^2 value implies a better fit. Similar results were obtained from fits done in k, q, and R-spaces.

Table S1. Crystal data and structure refinement details for **C1**.

	C1: C_{58} H_{55} Cl_2 Cu_2 N_9 O_4
FW/uma	1140.09
Crystal System	Triclinic
Space Group	$P^{-}1$
a (Å)	12.1101(15)
b (Å)	15.0255(18)
c (Å)	15.7251(19)
a (°)	75.136(1)
b (°)	67.643(1)
g (°)	87.203(2)
V (Å ^{3})	2553.9 (5)
Z(Z')	2
d (g cm^{-3})	1.483
m (mm^{-1})	1.00
F(000)	1180.0
q range	2.5–28.6
hkl range	$-14 \leq h \leq 14$
	$-18 \leq l \leq 18$
	$-19 \leq k \leq 19$
N_{tot}, N_{uniq} (R_{int}), N_{obs}	91681, 10027 (0.052), 7709
Ref. Parameters	697
R1, wR2 (obs)	0.050, 0.159
Max. and min Dr e $Å^{-3}$	1.27 and -0.98

EXAFS fit parameters for C1-C3

Table S2. Overview of the applied EXAFS fit parameters for **C1-C3** in solution phase.

Sample	**Fit**	**Region**	**Shell, N**	**R, Å**	**E_0**	**ss.^{2} (10^{-3})**	**R-factor**	**Reduced Chi-square**
C1	1	I	Cu-N, 4	2.01(3)	-0.3 (2.3)	8.6(2.2)	0.0094	1669
C2	2	I	Cu-N, 4	2.00(2)	-0.6(2.2)	7.9(2.0)	0.0083	1553
C3	3	I	Cu-N, 4	2.02(1)	3.9(1.3)	7.5(1.1)	0.0025	662
C1 Reconstructed Laser on state	4	I	Cu-N, 4	1.95(1)	-0.3*	8.6*	0.0164	12
C2 Reconstructed Laser on state	5	I	Cu-N, 4	1.95(1)	-0.6*	7.9*	0.0107	25
C3 Reconstructed Laser on state	6	I	Cu-N, 4	1.97(1)	3.3*	8.5*	0.0100	33

***** Region I corresponds to the fit between 1.1- 2.1 Å, in apparent distance scale for **C1-C3.** The reconstructed excited state of **C1, C2 and C3** corresponds to the substraction of the EXAFS data of the "Laser ON" states from the ground/ "Laser off" states.

Determination of Photon flux and ruling out possibilities of multi-photon effects

Multi-photon excitations are unlikely to occur under our experimental conditions considering the relatively long laser pulse width (1.6 ps) and low laser photon density. The photon flux (number of photons/pulse/molecule) was calculated in this case to be ~0.8, showing that the measurements reported in the manuscript were carried out in the linear regime. We also clarify that due to the dilute solution of the copper photosensitizers **C1-C3** (2 mM) hereby used, two-photon excitation process can be ruled due to the small cross section.

Table S3: Parameters employed in the calculation of the photon flux

Concentration [mol/L]	2×10^{-3} mol
Pump beam depth	650 µm (cylindrical jet)
Laser spot size	170 µm (V) x 750 µm (H)
Maximum effective area corresponding to the central plane of the cylindrical jet	170 µm (V) x 650 µm (H)
Volume of illuminated area	5.641×10^{7} um^3
Molecules in illuminated area	6.794×10^{13}
Pulse energy	~ 42 µJ
Excitation wavelength	400 nm
Photons/Pulse	8.458×10^{13}
Photons/Pulse on portion of cylindrical sample jet	5.757×10^{13}
Photon flux Photons/pulse/molecule	~0.8

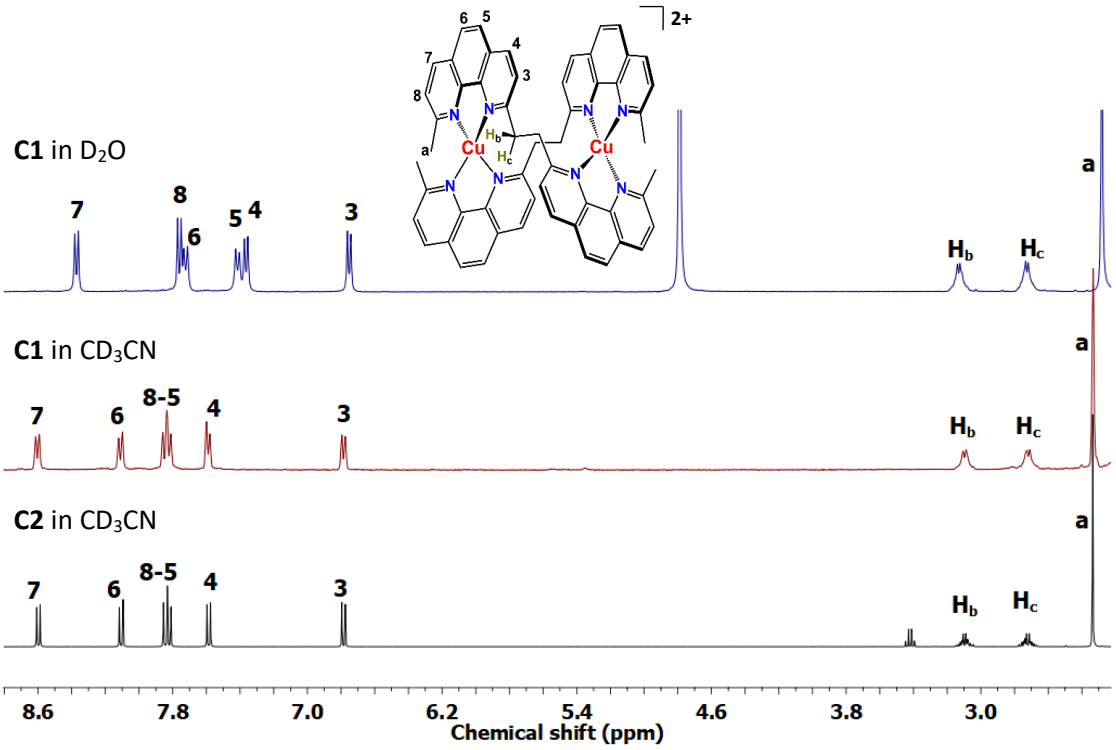

Figure S1. ^{1}H-NMR spectrum of **C1** in D_2O (top) and CD_3CN (middle) and **C2** in CD_3CN (bottom) at 298K.

In deuterated water (top), the ^{1}H-NMR spectra of **C1** shows in the aromatic region between 6.5 and 8.5 ppm the characteristic pattern of signals for disubstituted phenanthrolines. The protons of the aliphatic spacer appear as two pseudo-doublets (3.19 and 2.67 ppm), in agreement with their diastereotopic behavior due to the helical folding of the ligands around the copper atoms, which is indicative of a helical conformation. The existence of a single set of well-defined resonances implies that the four phenanthroline moieties are equivalent each other (*D2* symmetry), indicating that the intermolecular interactions observed in the crystal structure of **C1** are lost in solution. The same can be concluded from the spectra of **C1** (middle) and **C2** (bottom) in deuterated acetonitrile, where the protons of the ligands in both compounds have the same chemical environment, irrespective of the counterion's nature.

C1: ^{1}H-NMR (400 MHz, **D_2O**) δ ppm: 8.37 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.41 (d, *J* = 8.6 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 6.75 (d, *J* = 8.2 Hz, 1H), 3.19 – 3.07 (m, 1H), 2.79 – 2.67 (m, 1H).
C1: ^{1}H NMR (400 MHz, **CD_3CN**) δ ppm: 8.60 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 8.9 Hz, 1H), 7.86 - 7.81 (m, 2H), 7.59 (d, *J* = 7.9 Hz, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 3.12 - 3.04 (m, 1H), 2.75 - 2.66 (m, 1H), 2.33 (s, 3H).
C2: ^{1}H NMR (400 MHz, **CD_3CN**) δ 8.60 (d, *J* = 8.3 Hz, 1H), 8.11 (d, *J* = 8.9 Hz, 1H), 7.86 – 7.80 (m, 2H), 7.59 (d, *J* = 8.3 Hz, 1H), 6.79 (d, *J* = 8.3 Hz, 1H), 3.15 – 3.04 (m, 1H), 2.78 – 2.66 (m, 1H), 2.34 (s, 3H).

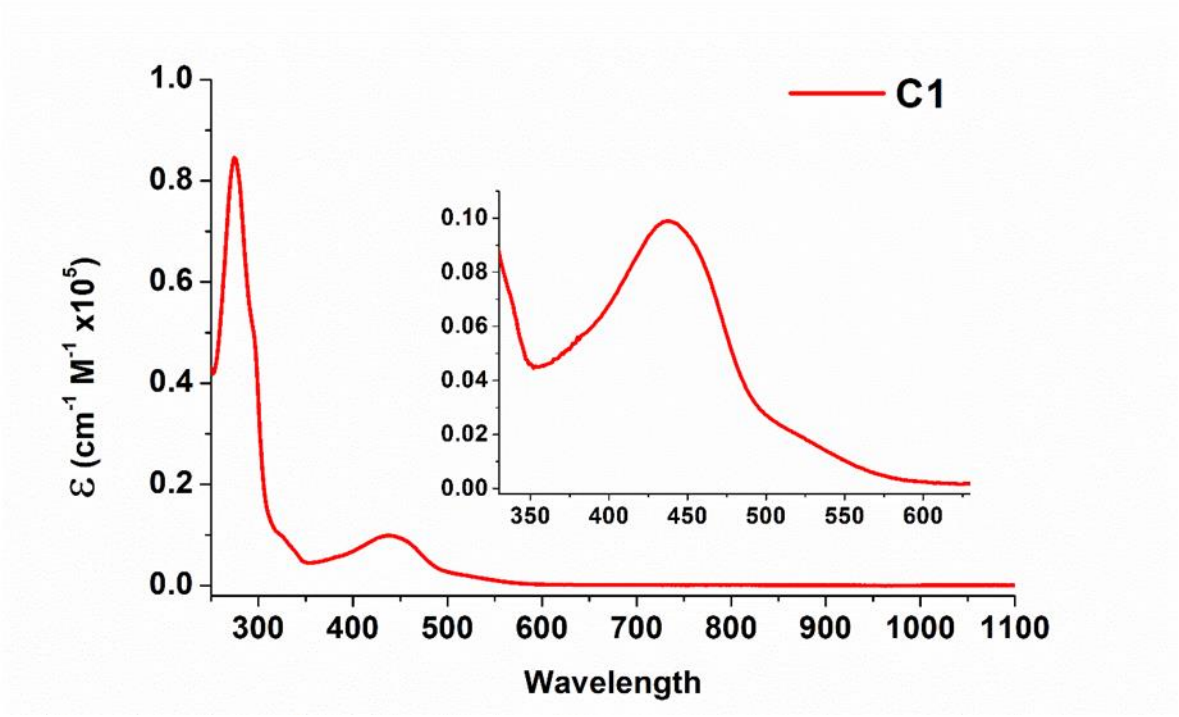

Figure S2. UV-vis spectrum of **C1** in H_2O at 298K. Inset: MLCT band.

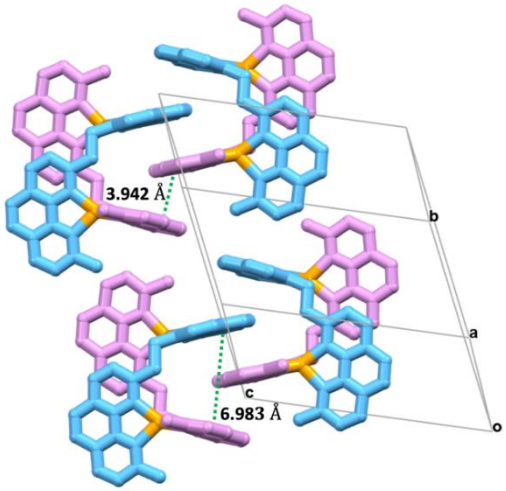

Figure S3. Crystal packing of **C1**. Distances between stacked phenanthroline rings are presented. The ligands are coloured to highlight the chirality *M* or *P* of the molecules. Ellipsoids are at a 50% of probability. Protons are omitted for clarity.

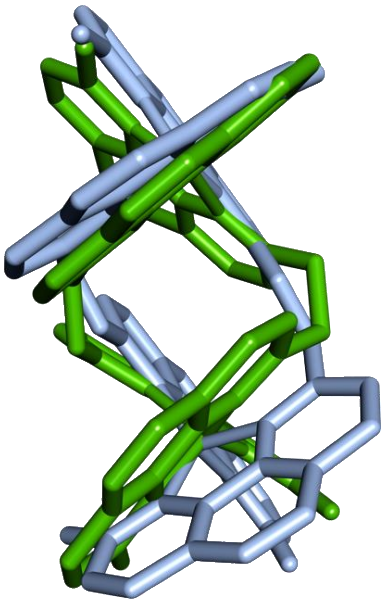

Figure S4: Overlay of the structures of *M*-**C1** (green) and *M*-**C2** (light blue). Superimposition was carried out considering the highest coincidence in the Cu-N_4 cores of both complexes.

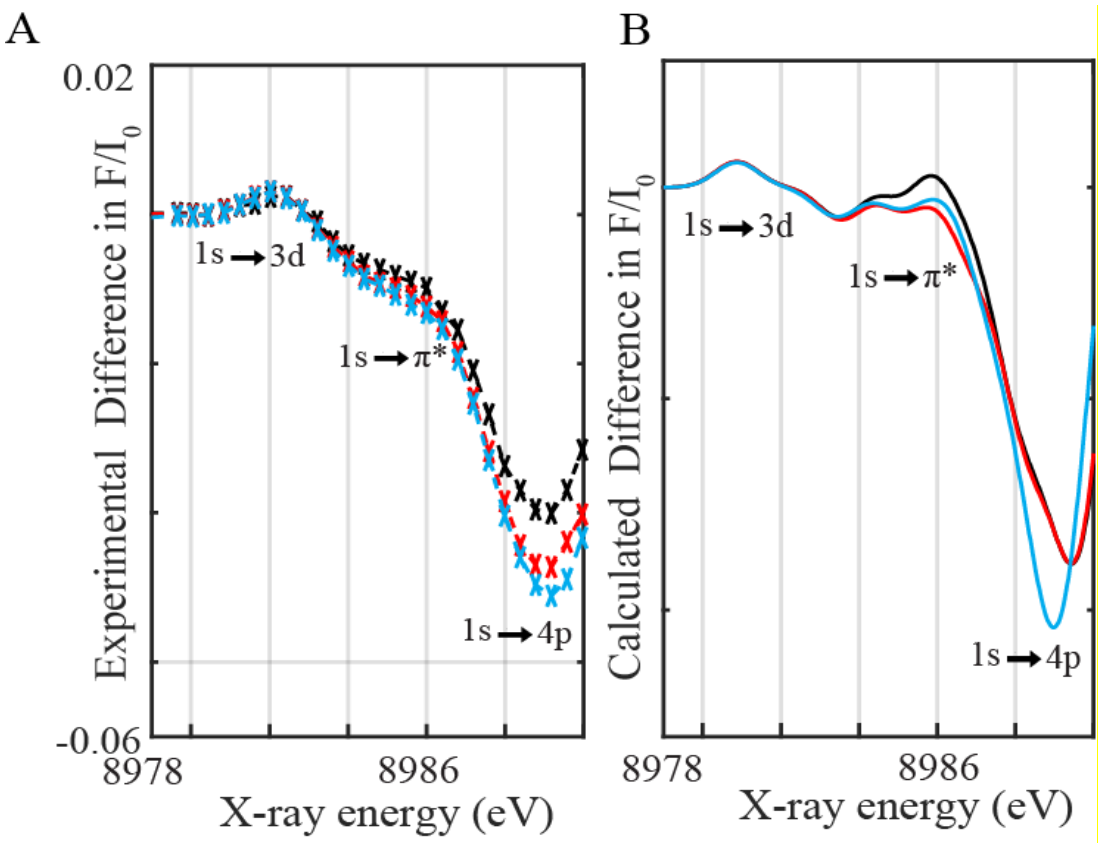

Figure S5 A. Experimental and **B**. Calculated TD-DFT transient XAS spectra of **C1-C3** over the pre-edge and part of the rising-edge region.

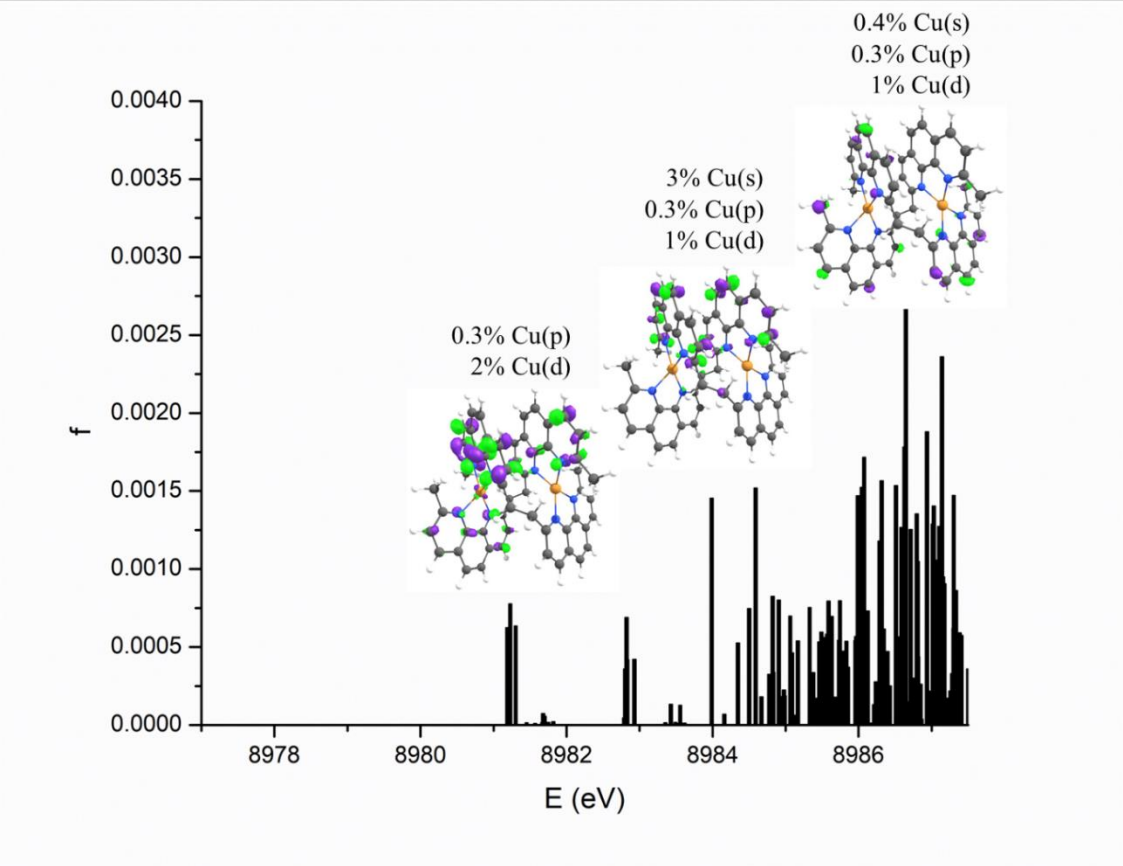

Figure S6. First 160 vertical electronic transitions (black bars) from the 1s orbitals of the copper(I) centers calculated by means of TDDFT for the compound **C1** at the **ground state** geometry. Most contributing orbitals of transitions with high oscillator strength are shown with its respective composition of orbitals of the copper atoms (s, p, d).

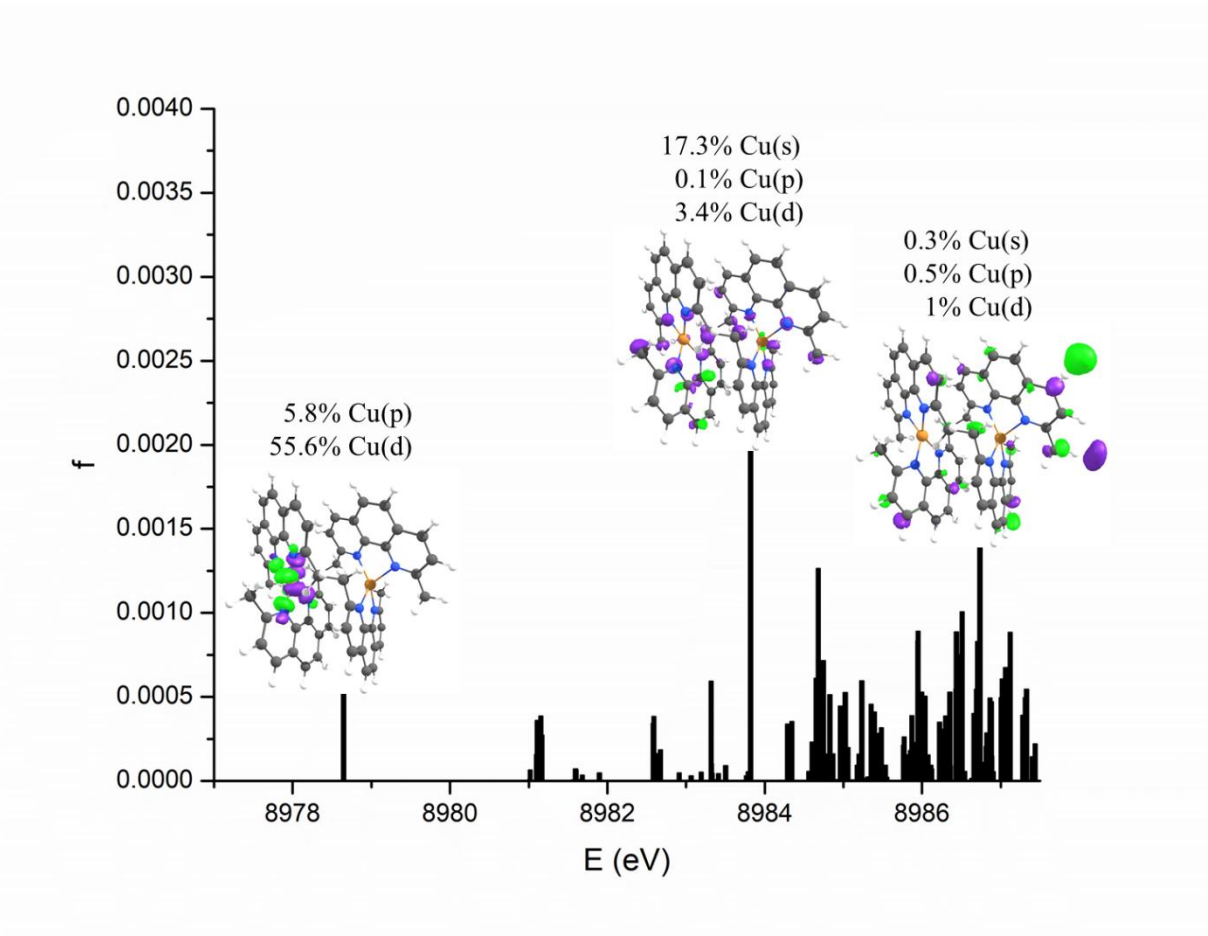

Figure S7. First 160 vertical electronic transitions (black bars) from the 1s orbitals of the copper(I) centers calculated by means of TDDFT for the compound **C1** at the **triplet state** geometry. Most contributing orbitals of transitions with high oscillator strength are shown with its respective composition of orbitals of the copper atoms (s, p, d).

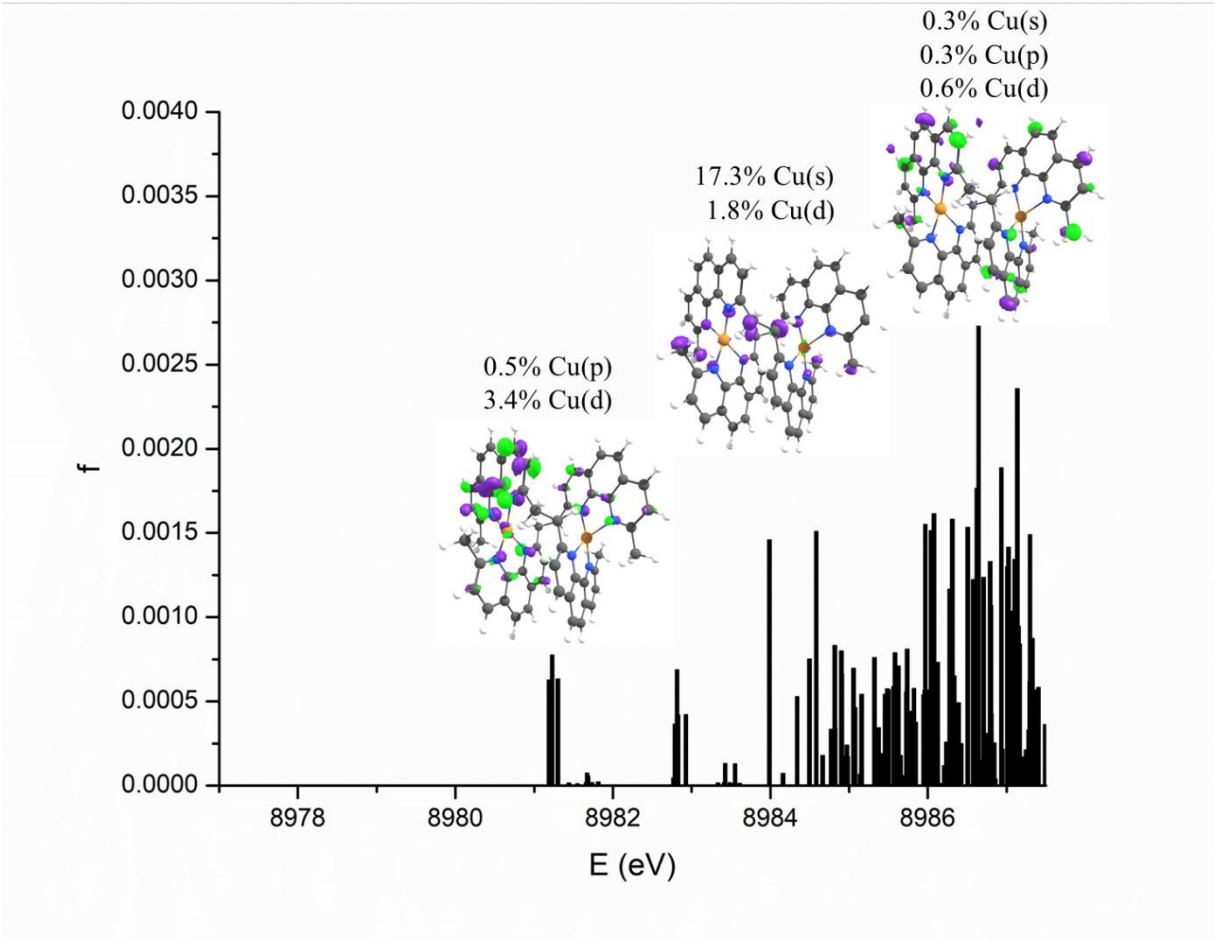

Figure S8. First 160 vertical electronic transitions (black bars) from the 1s orbitals of the copper(I) centers calculated by means of TDDFT for the compound **C2** at the **ground state** geometry. Most contributing orbitals of transitions with high oscillator strength are shown with its respective composition of orbitals of the copper atoms (s, p, d).

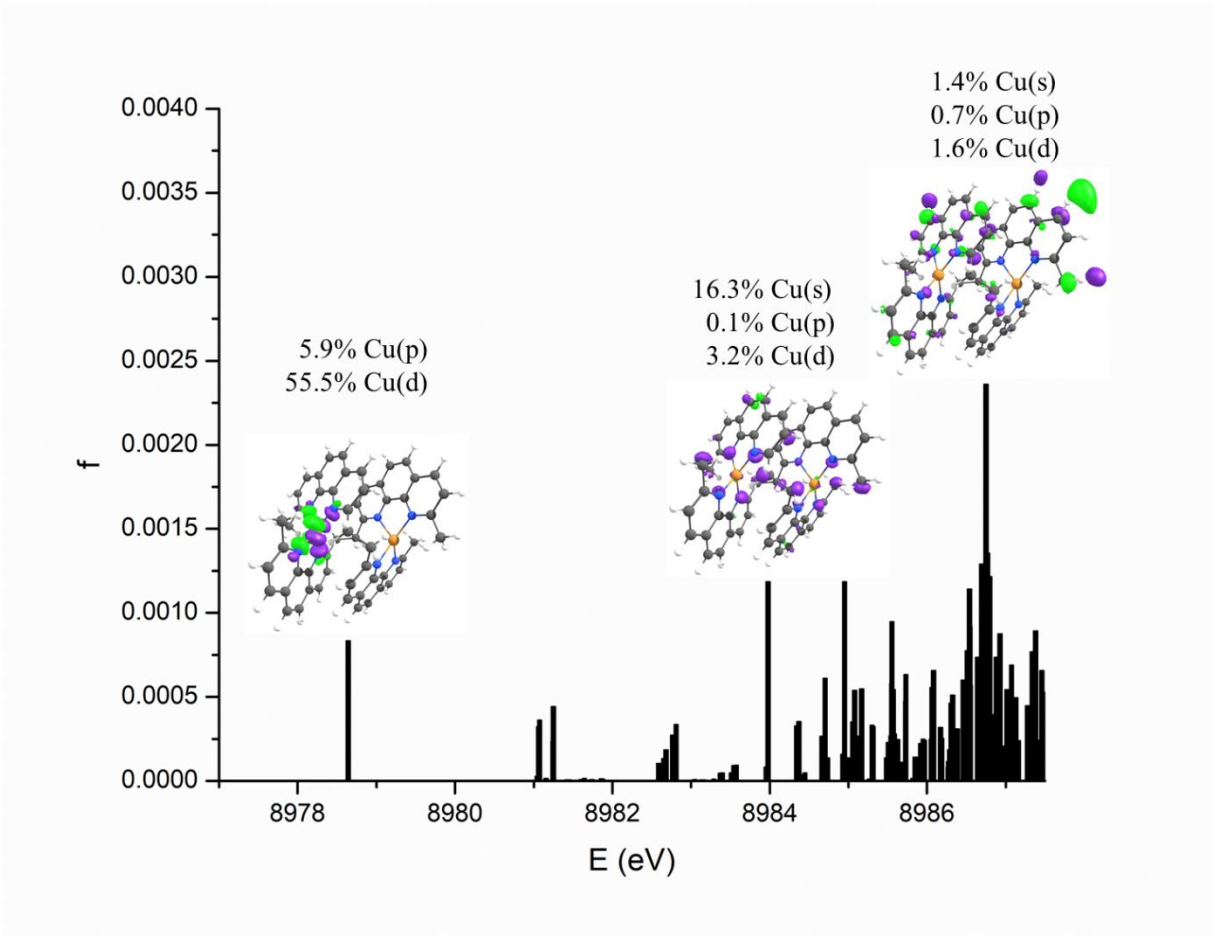

Figure S9. First 160 vertical electronic transitions (black bars) from the 1s orbitals of the copper(I) centers calculated by means of TDDFT for the compound **C2** at the **triplet state** geometry. Most contributing orbitals of transitions with high oscillator strength are shown with its respective composition of orbitals of the copper atoms (s, p, d).

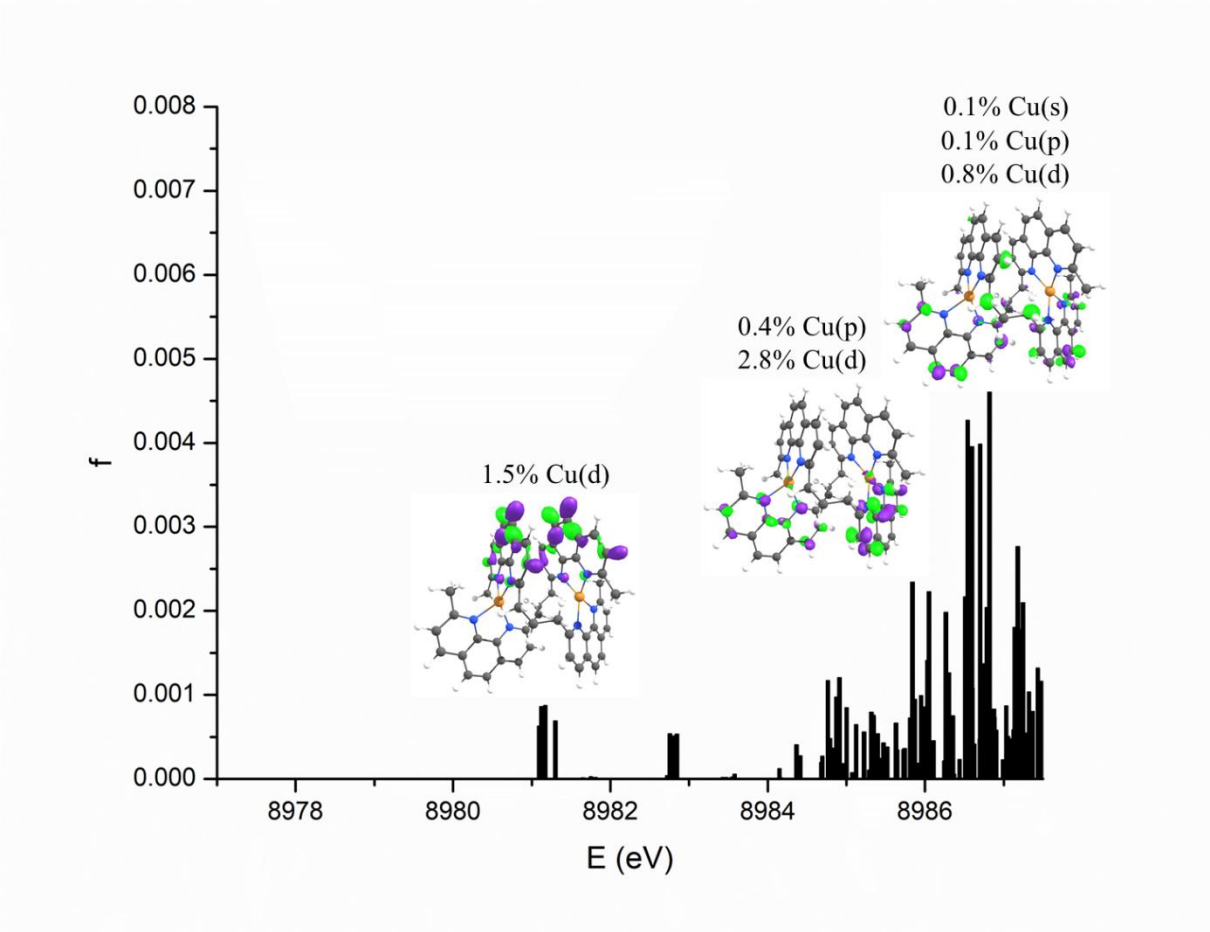

Figure S10. First 160 vertical electronic transitions (black bars) from the 1s orbitals of the copper(I) centers calculated by means of TDDFT for the compound **C3** at the **ground state** geometry. Most contributing orbitals of transitions with high oscillator strength are shown with its respective composition of orbitals of the copper atoms (s, p, d).

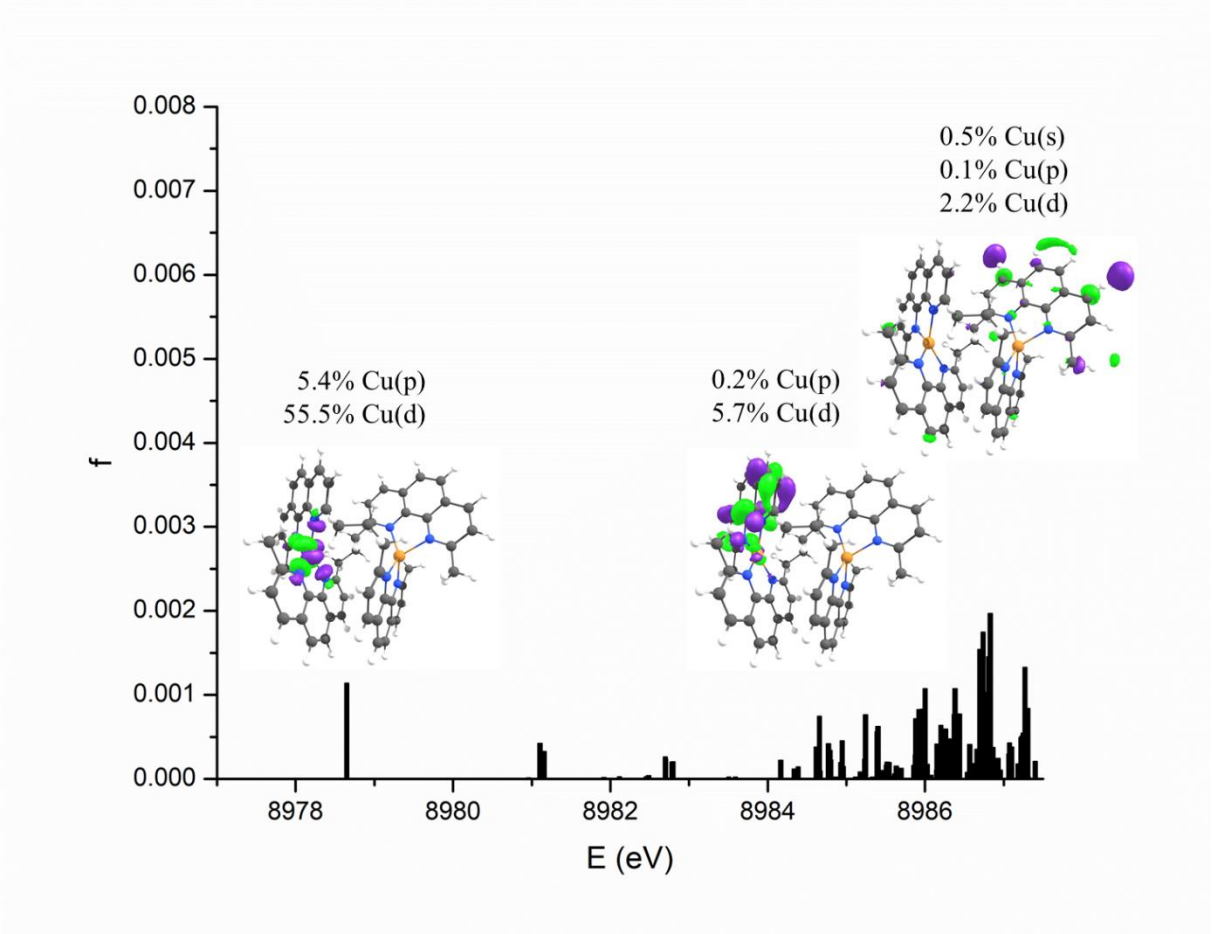

Figure S11. First 160 vertical electronic transitions (black bars) from the 1s orbitals of the copper(I) centers calculated by means of TDDFT for the compound **C3** at the **triplet state** geometry. Most contributing orbitals of transitions with high oscillator strength are shown with its respective composition of orbitals of the copper atoms (s, p, d).

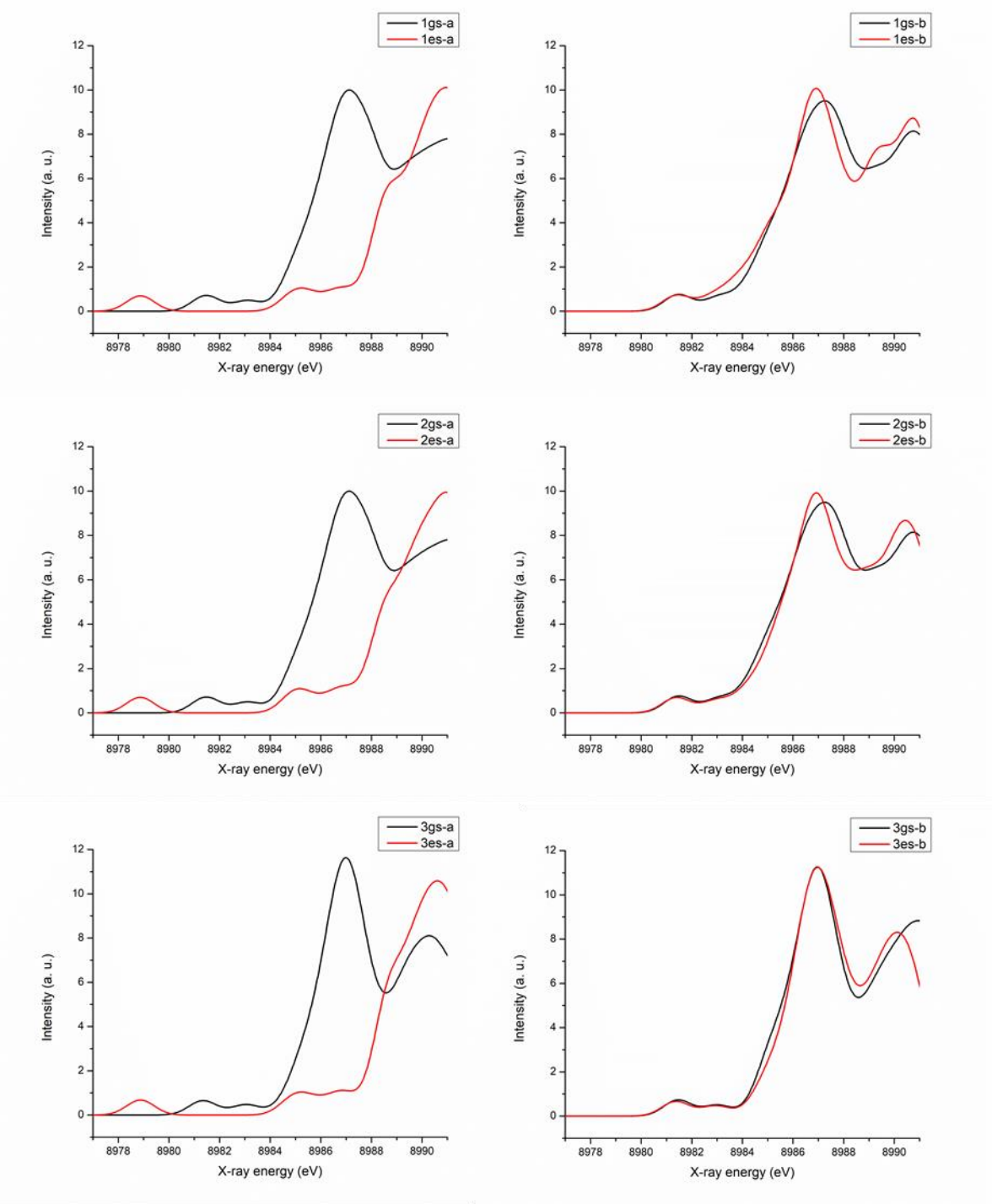

Figure S12. Calculated TD-DFT XAS spectra for each copper atom (denoted as a and b). Black and red lines correspond to the ground and excited state geometries, respectively.

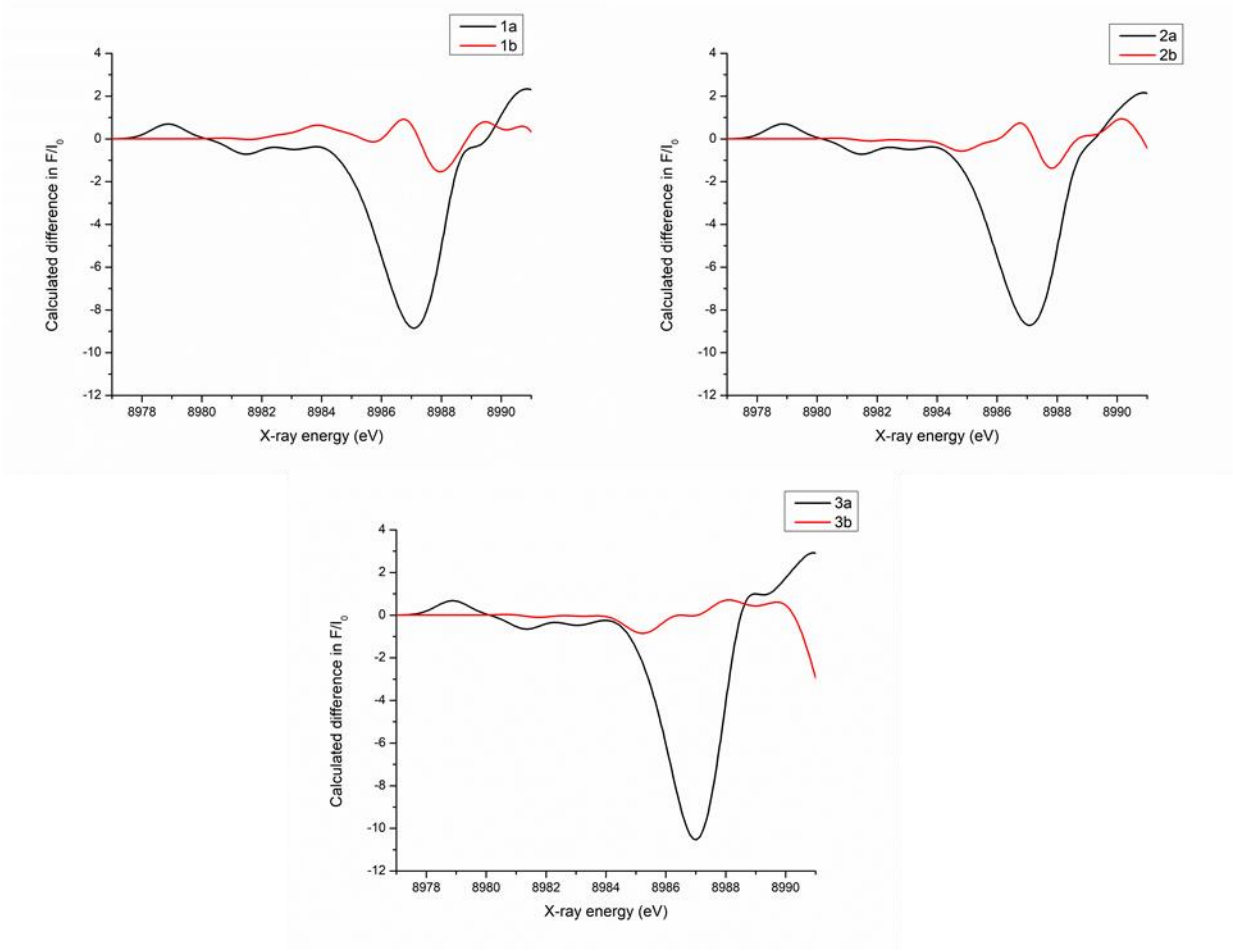

Figure S13. Calculated TD-DFT transient XAS spectra for each copper atom where black and red lines are referred to the copper atoms denoted as a and b, respectively.

The $[Cu^{I}(L_4)_2](ClO_4)_2$ complex previously reported by Pal[4], Lange[5] et al was used as a reference complex where L_4 is a bis-schiff base ligand with alkyl spacers (L= 4-CH_2-). This dimeric complex dissociates in acetonitrile solution as previously reported[5, 6] yielding the monometallic complex $[Cu^{I}(L_4)]^{+}$. In the presence of tetrachloroethane, CCL_4, the monomeric complex oxidizes spontaneously.

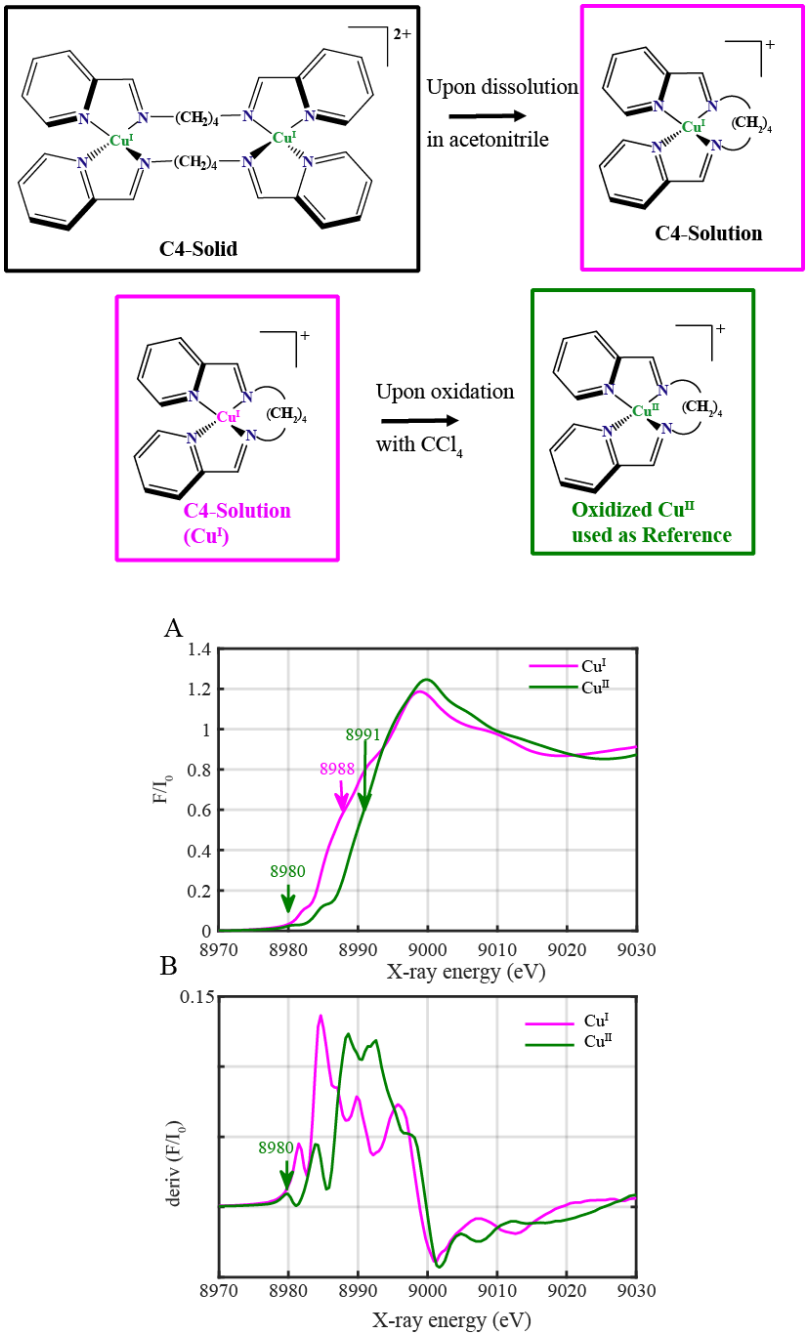

Figure S14. Top. General structure of dimeric[4] and monomeric[5, 6] reference Cu^{I} and oxidized Cu^{II} complexes employed for determination of excited state fraction. Cu^{I} was oxidized with CCL_4 to

generate the oxidized Cu^{II} reference complex B**ottom A**. Normalized **B**. Normalized Derivative Cu K-edge XANES of Cu^{I} and Cu^{II} monomeric reference complexes measured in solution.

The formation of pure Cu^{II} in the oxidized reference compound illustrated in Figure S14B is characterized by a 3 eV positive shift from the pure Cu^{I} complex at normalized absorption 0.6 , reflecting the higher ionization energy required for ejecting a core 1s electron from a more positively charged ion. A clear pre-edge feature at 8980 eV characteristic of Cu^{II} formation is also observed in the oxidized reference compound. Previously reported $[Cu(dmp)_2]^+$ complexes[7-10] (where dmp = 2,9-dimethyl-1,10,phenanthroline with similar coordination environments show similar relative chemical shift in energy of around 3 eV thus confirming the presence of pure Cu^{II} in the reference oxidized complex.

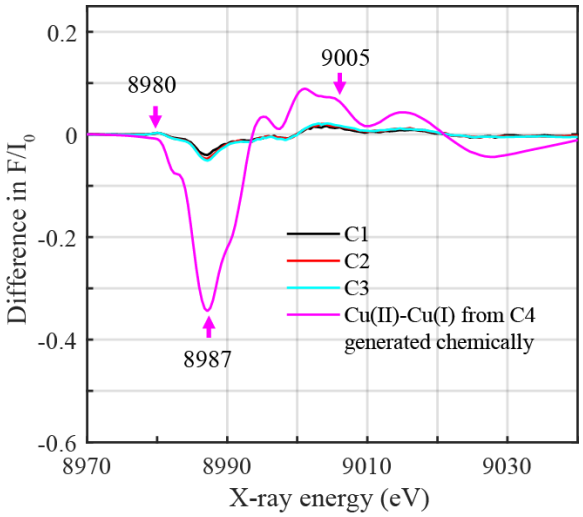

Figure S15: Determination of Excited State fraction by comparison with reference monomeric complex[6] chemically oxidized with CCl_4. The excited state fractions of **C1**, **C2** and **C3** were determined by comparing the negative maximum of the transient signal at 8987 eV with the chemically oxidized Cu(II) derivative of the reference complex. Using this strategy, a proportion of the excited state of 11.6 %, 13.7 % and 14.7 % were determined for **C1**, **C2** and **C3** respectively.

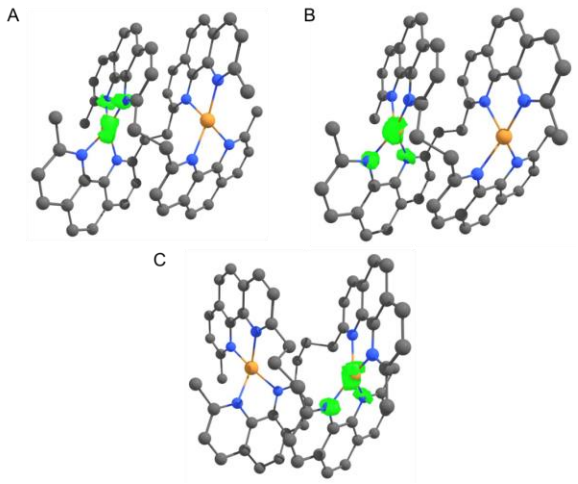

Figure S16. Spin density isosurface calculated for the compounds **C1** (A), **C2** (B) and **C3** (C) at the triplet state geometry. Hydrogen atoms are omitted for clarity.

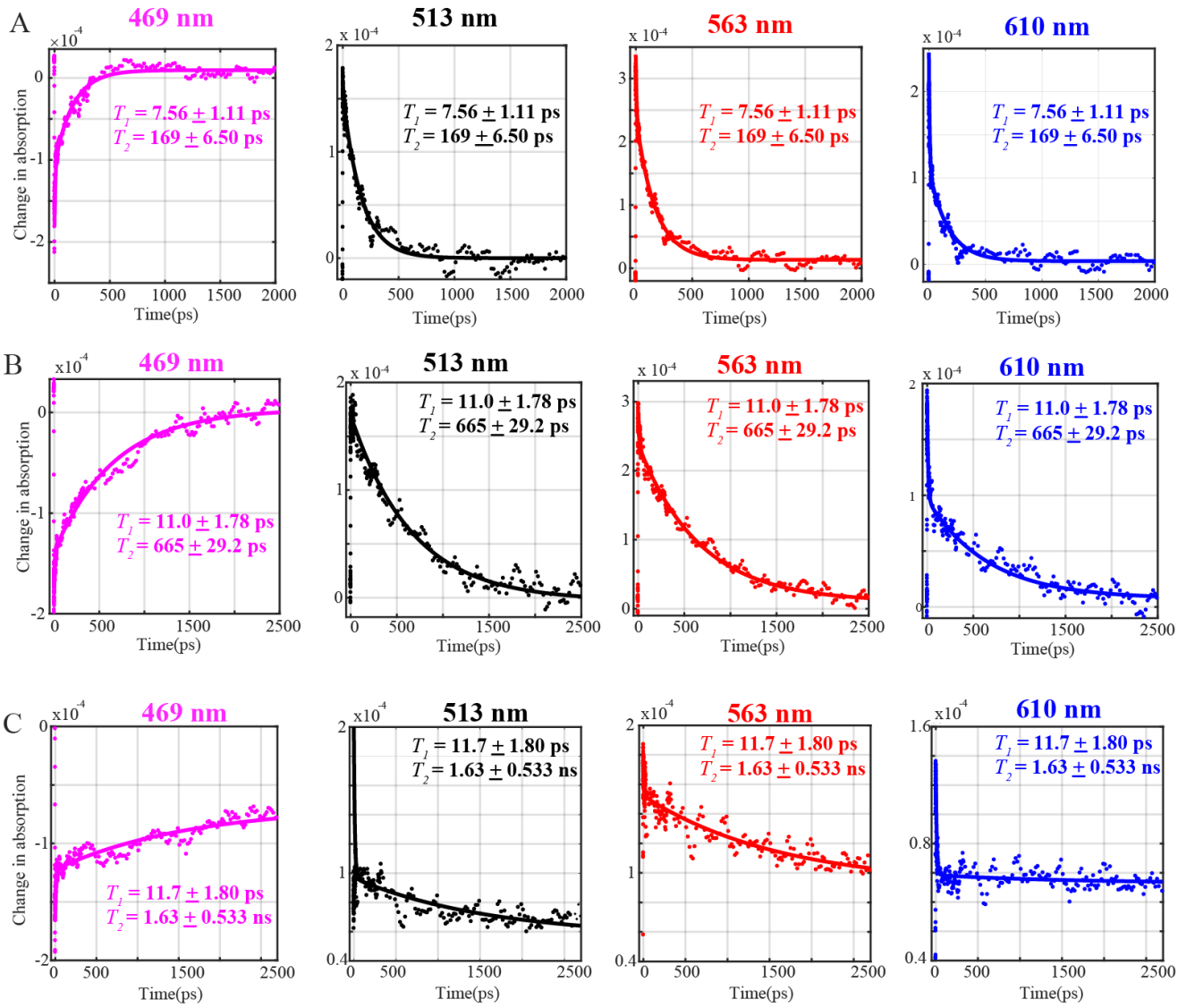

Figure S17. Global kinetic decay profiles of the transient absorption spectra at λ = 469 nm, 513 nm, 563 nm and 610 nm after excitation at λ_{exc} = 410 nm of **A. C1**, **B. C2** and **C. C3**. The solid lines are fittings to the decay kinetics and T_1 and T_2 are the resulting lifetimes.

Appendix:

Geometry optimizations were performed by means of Density Functional Theory using the B3LYP[11, 12] functional, Def2-TZVP[13, 14] basis set and the D3BJ[15] dispersion correction. The gas phase calculations were modeled without the polarizable continuum model[16] (PCM). However solvent effects with the PCM model were taken into considerations for comparisons to the ground and excited state structures in solution. The PCM model parameters included water for **C1** and acetonitrile for **C2** and **C3.** The code of each geometry includes the spin multiplicity, where singlets and triplets are models of the ground and excited states, respectively.

Complex **C2** is not included since in gas phase as it is the same in gas phase as in complex **C1**.

C1/C2-Singlet-gas

Cu	12.054475	2.183451	3.715154
Cu	12.144837	-3.203599	5.452892
N	13.059579	1.363690	2.119659
N	12.940662	3.415058	5.128689
N	13.108854	-1.554131	6.259863
C	10.332298	0.358303	5.503277
N	13.145948	-4.821690	4.614654
N	11.213802	1.350138	5.412661
N	11.352493	-3.291615	7.366776
N	10.983581	-3.434211	3.759050
C	9.867518	-2.794380	3.424279
C	12.527380	3.102782	6.378471
N	10.854059	2.924633	2.191726
C	11.308697	2.529335	0.980211
C	12.622898	-5.142246	3.406906
C	12.859059	-1.448129	7.586860
C	11.885556	-2.336531	8.162333
C	11.567934	2.041054	6.522074
C	12.477085	1.692164	0.942109
C	13.137729	-6.181897	2.607343
C	11.466083	-4.414628	2.958862
C	13.968844	-0.719475	5.682581
C	14.169776	0.631921	2.127219
C	12.990238	3.780344	7.524050
C	10.846698	-4.767983	1.742025
C	11.521810	2.466889	8.937641
C	11.045320	1.748334	7.797589
C	9.725051	0.046570	6.731530
C	10.065492	-0.402853	4.230839
C	14.172046	-5.517692	5.095602
C	10.437901	-4.126149	7.853609
C	14.768200	0.352713	3.477014

C	14.094688	-0.837712	4.186448
C	12.468996	3.430011	8.809726
C	11.517941	-2.180653	9.513432
C	9.785606	3.711157	2.274957
C	9.372934	-1.767637	4.403472
C	10.078999	0.731039	7.868955
C	12.509549	-6.490881	1.359937
C	9.193835	-3.085610	2.226002
C	14.442950	0.342084	7.791246
C	13.487466	-0.486214	8.403338
C	9.681497	-4.061819	1.389414
C	13.949773	4.790485	7.324154
C	12.991475	1.267909	-0.299690
C	10.695198	2.920602	-0.225749
C	12.336460	1.671811	-1.505736
C	14.249617	-6.883485	3.111078
C	13.822106	4.395629	4.949446
C	14.753906	-6.559741	4.346551
C	11.236099	2.466340	-1.469248
C	9.120372	4.151223	1.113606
C	11.402912	-5.820687	0.949763
C	14.740380	0.162953	0.932299
C	12.152803	-1.172666	10.306704
C	10.533032	-3.054467	10.009839
C	14.679745	0.225132	6.443135
C	14.360310	5.093577	6.048591
C	13.115102	-0.375323	9.779215
C	14.154401	0.474827	-0.272460
C	10.001813	-4.019358	9.188522
C	9.569925	3.761202	-0.124266
H	9.254900	-4.708341	9.558173
H	10.208309	-2.966664	11.039201
H	11.858649	-1.068371	11.343619
H	13.606192	0.372390	10.387775
H	14.970722	1.079650	8.382066
H	15.398113	0.871545	5.963099
H	8.257819	4.796283	1.208535
H	9.069296	4.097480	-1.023599
H	10.752910	2.780602	-2.385650
H	12.743671	1.336287	-2.450825
H	14.588752	0.129143	-1.202099
H	15.646707	-0.425828	0.969508
H	15.084383	5.877605	5.874966
H	14.346266	5.330458	8.174823
H	12.833646	3.965276	9.677369
H	11.114107	2.217592	9.908350

H	9.632502	0.479803	8.822218
H	8.991232	-0.743035	6.786084
H	15.592533	-7.103046	4.758582
H	14.687139	-7.683820	2.527629
H	12.924710	-7.287997	0.756828
H	10.918960	-6.079270	0.016812
H	9.168203	-4.306580	0.467999
H	8.286957	-2.550538	1.978866
C	9.336140	4.107840	3.647529
H	8.389041	4.643111	3.623782
H	9.230019	3.224690	4.278792
H	10.082625	4.752598	4.118106
C	14.203019	4.724935	3.539386
H	14.751714	3.895189	3.087243
H	13.306559	4.881413	2.937332
H	14.824675	5.616344	3.487126
C	9.895795	-5.169917	6.928238
H	10.711826	-5.674579	6.410046
H	9.297822	-5.906942	7.460925
H	9.269148	-4.707612	6.160731
C	14.655012	-5.179959	6.473314
H	13.873415	-5.401493	7.203969
H	15.542277	-5.751305	6.737902
H	14.879720	-4.115008	6.556599
H	15.841527	0.184802	3.385784
H	14.618354	1.255562	4.069362
H	13.081955	-0.972073	3.804097
H	14.618058	-1.767484	3.946000
H	8.290581	-1.661373	4.323724
H	9.596523	-2.161814	5.394716
H	11.030136	-0.536047	3.740380
H	9.485416	0.231964	3.554621

C1/C2-triplet-gas

Cu	11.844802	2.462650	3.576266
Cu	12.097619	-3.509389	5.698361
N	12.786121	1.407389	2.058129
N	12.842887	3.666635	4.932312
N	12.760464	-1.742669	6.383683
C	10.149366	0.715721	5.468675
N	12.963107	-5.158978	4.880218
N	11.032301	1.693671	5.317188
N	11.609341	-3.840807	7.586020
N	11.323796	-3.299965	3.863307
C	10.403034	-2.424321	3.443837

C	12.485152	3.376462	6.205614
N	10.778427	3.217596	1.979717
C	11.211192	2.700406	0.805256
C	12.684950	-5.222645	3.542129
C	12.681786	-1.730169	7.760259
C	12.023261	-2.803720	8.385211
C	11.503027	2.347802	6.409396
C	12.273483	1.732201	0.847599
C	13.228690	-6.213163	2.700073
C	11.809672	-4.243487	3.005103
C	13.438587	-0.751585	5.755306
C	13.788899	0.538847	2.140015
C	13.044822	4.034061	7.319928
C	11.453408	-4.272963	1.641191
C	11.678514	2.714683	8.827708
C	11.096493	2.026875	7.718991
C	9.664519	0.364339	6.742775
C	9.731630	-0.046775	4.238796
C	13.827984	-6.028694	5.417241
C	10.922580	-4.864971	8.120403
C	14.297267	0.246011	3.524314
C	13.386397	-0.752716	4.251924
C	12.617936	3.676383	8.637079
C	11.808635	-2.805814	9.784840
C	9.805636	4.123380	1.987063
C	9.739583	-1.575402	4.489165
C	10.137045	1.007061	7.858851
C	12.865946	-6.220297	1.315559
C	10.021400	-2.386371	2.097646
C	13.974864	0.287914	7.875228
C	13.244422	-0.694755	8.540817
C	10.554079	-3.289324	1.195546
C	14.013810	5.021961	7.057948
C	12.757370	1.172574	-0.353172
C	10.669415	3.082371	-0.436857
C	12.181156	1.578266	-1.597940
C	14.098333	-7.144851	3.288116
C	13.748261	4.611930	4.697664
C	14.400616	-7.039616	4.630561
C	11.180777	2.495782	-1.637002
C	9.213255	4.557298	0.784369
C	12.008457	-5.295938	0.809116
C	14.323451	-0.067493	0.990110
C	12.322074	-1.709854	10.550632
C	11.118025	-3.891469	10.326335
C	14.072239	0.243311	6.485445

C	14.358994	5.308321	5.759847
C	13.029520	-0.714603	9.957690
C	13.811167	0.244927	-0.247475
C	10.665719	-4.906278	9.490555
C	9.640648	4.044544	-0.415483
H	10.112925	-5.742462	9.894038
H	10.928801	-3.936581	11.391367
H	12.151588	-1.703071	11.619868
H	13.446858	0.089736	10.549803
H	14.442231	1.087074	8.433350
H	14.619948	1.015174	5.970342
H	8.424594	5.296444	0.818313
H	9.195104	4.375140	-1.345473
H	10.754333	2.807221	-2.582176
H	12.567823	1.143752	-2.511049
H	14.220214	-0.205426	-1.143349
H	15.145060	-0.764147	1.087475
H	15.094444	6.069798	5.539988
H	14.474038	5.552431	7.881799
H	13.057363	4.194349	9.480179
H	11.353431	2.448066	9.825123
H	9.789281	0.726866	8.844950
H	8.934744	-0.427560	6.838956
H	15.081197	-7.738164	5.095651
H	14.533276	-7.932074	2.686029
H	13.283266	-6.989408	0.678463
H	11.723558	-5.325886	-0.234692
H	10.254873	-3.266551	0.155463
H	9.288035	-1.658078	1.778560
C	9.386713	4.670734	3.316575
H	8.436648	5.198092	3.254061
H	9.305571	3.865268	4.047282
H	10.138628	5.371618	3.689212
C	14.086069	4.897042	3.267446
H	14.576831	4.032232	2.814350
H	13.175602	5.083313	2.695537
H	14.746092	5.756622	3.171628
C	10.422309	-5.935980	7.201624
H	11.240855	-6.465412	6.713490
H	9.822378	-6.662677	7.745305
H	9.805902	-5.499762	6.411351
C	14.177184	-5.896259	6.867221
H	13.356703	-6.224364	7.507599
H	15.047640	-6.501654	7.108926
H	14.389738	-4.856895	7.121311
H	15.319415	-0.131431	3.486775

H	14.309562	1.197107	4.054353
H	12.355657	-0.537010	3.966110
H	13.590085	-1.762389	3.885131
H	8.714126	-1.940325	4.597166
H	10.231372	-1.779064	5.437716
H	10.412842	0.223671	3.431876
H	8.738507	0.281954	3.922040

C3-singlet-gas

Cu	3.747683	5.455341	10.187134
Cu	2.859362	-0.028242	8.495926
N	5.253418	5.975377	8.887639
N	5.080997	3.915371	10.663086
N	1.103779	0.612677	9.342410
N	1.564251	-1.274784	7.457131
N	2.920964	6.528915	11.727533
N	1.804948	5.596916	9.434323
N	4.294791	1.116474	7.497988
N	4.519147	-0.736721	9.469413
C	5.295187	6.993968	8.033231
C	6.407211	7.187711	7.192014
H	6.414334	8.024519	6.507214
C	7.482546	6.338936	7.271918
H	8.357609	6.498286	6.653999
C	7.457768	5.267281	8.184824
C	8.559193	4.378360	8.377549
H	9.456530	4.533907	7.791711
C	8.496596	3.383329	9.296651
H	9.342043	2.729241	9.460722
C	7.316839	3.174597	10.075866
C	7.200387	2.147190	11.029354
H	8.022842	1.459842	11.177188
C	6.054688	2.042711	11.775914
H	5.954212	1.271623	12.528143
C	5.008184	2.967707	11.596345
C	6.210891	4.033712	9.916845
C	6.293871	5.113322	8.965792
C	4.125841	7.926535	8.002119
H	4.379919	8.860551	7.504488
H	3.782037	8.139380	9.014210
H	3.289517	7.472295	7.465665
C	3.803871	2.924936	12.498619
H	3.400759	3.935028	12.580099
H	4.135817	2.618608	13.493021

C	2.678532	1.979138	12.052217
H	3.040662	0.947733	12.036705
H	1.885400	2.024806	12.802140
C	2.123166	2.357825	10.678725
H	1.859514	3.416804	10.688197
H	2.905140	2.232375	9.928233
C	0.921493	1.577991	10.236342
C	-0.368568	1.902239	10.695341
H	-0.488694	2.688879	11.428425
C	-1.462778	1.239722	10.195360
H	-2.460531	1.492036	10.532009
C	-1.287391	0.234517	9.223374
C	-2.369047	-0.480159	8.619494
H	-3.378506	-0.249085	8.934435
C	-2.137900	-1.427568	7.674045
H	-2.960201	-1.966394	7.220602
C	-0.806717	-1.736147	7.251327
C	-0.505101	-2.698907	6.268276
H	-1.306829	-3.254872	5.799200
C	0.802785	-2.920993	5.911940
H	1.051928	-3.655753	5.158631
C	1.835097	-2.184555	6.526002
C	0.280875	-1.048063	7.825863
C	0.035898	-0.049019	8.830960
C	3.273112	-2.386401	6.159052
H	3.713293	-1.446017	5.821296
H	3.388259	-3.128178	5.371337
H	3.843430	-2.714502	7.031025
C	3.509849	6.975019	12.833354
C	2.766362	7.633046	13.831598
H	3.269661	7.980481	14.723191
C	1.421496	7.844051	13.659566
H	0.841522	8.357629	14.415698
C	0.791745	7.407469	12.478041
C	-0.588283	7.639800	12.190774
H	-1.189117	8.158819	12.926610
C	-0.345223	6.550567	10.039665
C	-0.848223	6.138092	8.790455
H	-1.876206	6.355148	8.528286
C	-0.021456	5.491222	7.907873
H	-0.386373	5.190102	6.935393
C	1.316845	5.220415	8.257384
C	1.009763	6.269828	10.307604
C	1.594786	6.732077	11.537331
C	4.983212	6.752691	12.977741
H	5.188612	5.722840	13.281688

H	5.412187	7.413831	13.727713
H	5.486273	6.916484	12.024766
C	2.229485	4.514013	7.292980
H	3.247444	4.574010	7.678645
H	2.206139	5.047370	6.337354
C	1.840393	3.049735	7.051644
H	0.819741	2.998144	6.665027
H	1.836606	2.508957	7.992889
C	2.756588	2.324989	6.055664
H	2.295028	1.364776	5.809683
H	2.816539	2.896309	5.127688
C	4.151845	2.032311	6.543191
C	5.274654	2.650967	5.959091
H	5.127144	3.408723	5.201918
C	6.540977	2.257974	6.317636
H	7.411756	2.702792	5.854065
C	6.707387	1.251831	7.285382
C	7.984987	0.741660	7.674976
H	8.865476	1.130891	7.181283
C	8.093697	-0.203418	8.641646
H	9.063204	-0.585305	8.936498
C	6.932470	-0.717657	9.298253
C	6.985561	-1.665969	10.336487
H	7.944495	-2.038707	10.674985
C	5.820677	-2.113014	10.911258
H	5.843337	-2.842498	11.709098
C	4.580357	-1.638327	10.444626
C	5.656768	-0.263611	8.910599
C	5.538814	0.734741	7.880334
C	3.285929	-2.143133	11.000162
H	2.594731	-1.317031	11.169535
H	3.432546	-2.688313	11.930721
H	2.809192	-2.817691	10.284038
C	-1.132512	7.240848	11.012840
H	-2.171288	7.446149	10.788734

C3-triplet-gas

Cu	3.759043	5.332907	10.100052
Cu	2.846890	0.126139	8.557015
N	5.099467	5.790852	8.700640
N	5.099297	3.972856	10.686613
N	1.078496	0.793424	9.360587
N	1.560209	-1.122216	7.504744
N	2.963127	6.168614	11.750203
N	1.906969	5.610072	9.345741

N	4.307408	1.205366	7.517091
N	4.491842	-0.597051	9.542081
C	5.101630	6.800623	7.808357
C	6.220327	7.046430	7.015811
H	6.188423	7.863456	6.309199
C	7.365853	6.270512	7.145478
H	8.237805	6.474139	6.537273
C	7.401416	5.252529	8.100293
C	8.554218	4.447086	8.363398
H	9.451064	4.630460	7.784912
C	8.535626	3.492183	9.326245
H	9.414994	2.895397	9.527326
C	7.366325	3.257479	10.117697
C	7.289248	2.287264	11.116511
H	8.139854	1.651549	11.319956
C	6.118684	2.161977	11.855855
H	6.042471	1.417892	12.636625
C	5.047995	3.027942	11.649670
C	6.227245	4.067107	9.896835
C	6.238165	5.039714	8.878397
C	3.887249	7.667498	7.696434
H	4.124503	8.581440	7.156676
H	3.505734	7.934114	8.682698
H	3.080809	7.163934	7.161760
C	3.832701	2.905154	12.531091
H	3.398802	3.886364	12.713668
H	4.162135	2.520069	13.496935
C	2.732576	1.973762	11.994398
H	3.148886	0.985838	11.789840
H	1.982146	1.852109	12.778683
C	2.067859	2.531233	10.735157
H	1.743926	3.550993	10.942551
H	2.804858	2.567130	9.931118
C	0.877300	1.761653	10.248049
C	-0.419263	2.095983	10.677441
H	-0.549060	2.888252	11.402733
C	-1.506651	1.436088	10.159214
H	-2.510012	1.693644	10.474569
C	-1.314308	0.426062	9.197004
C	-2.388924	-0.286236	8.577848
H	-3.402270	-0.048600	8.874853
C	-2.146311	-1.237772	7.640080
H	-2.963112	-1.774069	7.173912
C	-0.809174	-1.556337	7.245200
C	-0.495526	-2.528456	6.275183
H	-1.292570	-3.078689	5.791678

C	0.817559	-2.771003	5.953983
H	1.075845	-3.516740	5.214642
C	1.843605	-2.045224	6.590966
C	0.272102	-0.874382	7.838584
C	0.016134	0.134624	8.831248
C	3.287496	-2.269783	6.264382
H	3.705354	-1.387052	5.774268
H	3.423420	-3.124074	5.604385
H	3.862341	-2.431623	7.177144
C	3.570733	6.537311	12.886223
C	2.839197	7.150209	13.911892
H	3.351807	7.431848	14.820838
C	1.487495	7.389747	13.766486
H	0.920212	7.848081	14.565999
C	0.851492	7.064042	12.558475
C	-0.527286	7.324480	12.284471
H	-1.129547	7.782420	13.058447
C	-0.281764	6.425433	10.043040
C	-0.773516	6.110427	8.766791
H	-1.803038	6.331131	8.515975
C	0.067689	5.530041	7.839415
H	-0.296496	5.277379	6.853566
C	1.409073	5.269091	8.151319
C	1.079155	6.153142	10.294070
C	1.641372	6.459385	11.559183
C	5.038001	6.285973	13.041708
H	5.231805	5.266244	13.382909
H	5.462126	6.964527	13.778652
H	5.562125	6.418697	12.096297
C	2.289408	4.568194	7.155782
H	3.322718	4.611940	7.491258
H	2.234916	5.089408	6.196245
C	1.875325	3.103391	6.952436
H	0.857590	3.056351	6.559176
H	1.857824	2.587962	7.908458
C	2.799547	2.346457	5.990946
H	2.338435	1.380752	5.767588
H	2.875925	2.889386	5.047342
C	4.185441	2.071644	6.514503
C	5.318738	2.659857	5.920921
H	5.187169	3.381009	5.125933
C	6.577151	2.283930	6.322135
H	7.457065	2.708716	5.857230
C	6.723334	1.320739	7.335592
C	7.992248	0.820825	7.762753
H	8.881466	1.191421	7.270748

C	8.081597	-0.091766	8.761714
H	9.044538	-0.467581	9.084281
C	6.908058	-0.583245	9.413337
C	6.941516	-1.511480	10.470224
H	7.894254	-1.875452	10.834663
C	5.766256	-1.954419	11.026049
H	5.773872	-2.673246	11.833835
C	4.534873	-1.491365	10.525559
C	5.640337	-0.134597	8.995013
C	5.543118	0.833120	7.933770
C	3.231811	-2.010394	11.048611
H	2.506490	-1.202525	11.147049
H	3.353652	-2.507819	12.009209
H	2.810412	-2.735232	10.346528
C	-1.071339	7.017260	11.078061
H	-2.112675	7.231033	10.874607

C1-Singlet-PCM

Cu	11.975318	1.834274	3.703523
Cu	11.737265	-2.946092	5.534428
N	12.846902	1.074056	2.010265
N	13.035833	2.787660	5.188501
N	13.088689	-1.460686	6.177447
C	9.954910	0.185497	5.330571
N	13.110802	-4.420390	4.834372
N	10.997918	1.005875	5.320936
N	11.104818	-2.763907	7.476000
N	10.978826	-3.230155	3.659998
C	9.884020	-2.697233	3.125225
C	12.546401	2.467106	6.412013
N	10.684064	2.678007	2.303397
C	11.006178	2.272238	1.053540
C	12.941896	-4.600324	3.505696
C	13.025301	-1.329918	7.519182
C	11.935814	-1.972715	8.202063
C	11.430379	1.566570	6.476678
C	12.155012	1.419795	0.897722
C	13.839745	-5.351419	2.720676
C	11.788542	-4.002712	2.889085
C	14.057814	-0.867544	5.492950
C	13.957642	0.350586	1.898957

C	13.077803	2.999054	7.602604
C	11.535728	-4.239116	1.523312
C	11.365152	1.883812	8.905649
C	10.827770	1.295886	7.720157
C	9.281778	-0.112982	6.533453
C	9.505317	-0.357495	4.002971
C	14.161648	-4.952348	5.445998
C	10.048842	-3.318019	8.063501
C	14.700221	0.053136	3.170484
C	13.996361	-1.036580	3.999681
C	12.458830	2.686885	8.851505
C	11.759732	-1.743782	9.579524
C	9.633017	3.468463	2.494336
C	9.032517	-1.835227	4.006914
C	9.713742	0.433631	7.714348
C	13.572236	-5.543824	1.330221
C	9.551072	-2.908857	1.774041
C	15.005515	0.023971	7.518570
C	13.958945	-0.568614	8.250506
C	10.369176	-3.670783	0.976600
C	14.204427	3.835673	7.483382
C	12.538212	0.999420	-0.391899
C	10.275962	2.669733	-0.084312
C	11.765458	1.407843	-1.525205
C	14.965709	-5.886907	3.376262
C	14.078719	3.604801	5.087358
C	15.123049	-5.690343	4.725704
C	10.680978	2.212441	-1.377663
C	8.857830	3.915973	1.406058
C	12.455315	-5.024370	0.758005
C	14.404804	-0.105887	0.647892
C	12.716794	-0.956273	10.294356
C	10.620465	-2.314390	10.181116
C	15.054292	-0.122782	6.152337
C	14.702301	4.129047	6.238357
C	13.786522	-0.410342	9.660304
C	13.695961	0.204232	-0.488940
C	9.773327	-3.086726	9.426339
C	9.177395	3.524674	0.128360
H	8.895685	-3.537991	9.868218

H	10.421245	-2.135305	11.230503
H	12.562990	-0.796555	11.354186
H	14.507031	0.185877	10.205387
H	15.755350	0.607554	8.037364
H	15.844639	0.343626	5.583008
H	8.016111	4.569439	1.589936
H	8.595411	3.868147	-0.717574
H	10.105623	2.530887	-2.237975
H	12.073053	1.064782	-2.504781
H	14.029406	-0.143172	-1.458582
H	15.309653	-0.694548	0.592543
H	15.559706	4.777939	6.124260
H	14.659454	4.248368	8.374944
H	12.882502	3.107304	9.754601
H	10.896088	1.650624	9.852292
H	9.215625	0.198560	8.646006
H	8.429946	-0.777778	6.521552
H	15.973251	-6.103983	5.250352
H	15.691080	-6.457122	2.809842
H	14.275897	-6.122201	0.744691
H	12.243100	-5.189895	-0.290550
H	10.124701	-3.846846	-0.063505
H	8.649989	-2.461329	1.378487
C	9.304165	3.846844	3.905026
H	8.546844	4.627848	3.942515
H	8.926939	2.975564	4.446453
H	10.200460	4.189014	4.424946
C	14.566981	3.946627	3.713442
H	15.272076	3.188893	3.359138
H	13.732541	3.975352	3.013440
H	15.084039	4.905223	3.707239
C	9.140884	-4.167953	7.230637
H	9.685271	-4.609226	6.396525
H	8.683623	-4.955575	7.828709
H	8.331749	-3.557008	6.820231
C	14.291061	-4.733687	6.920155
H	13.312519	-4.784730	7.396712
H	14.954048	-5.469320	7.371152
H	14.703090	-3.741110	7.120358
H	15.724406	-0.238713	2.944135

H	14.739302	0.978131	3.745251
H	12.937828	-1.071677	3.741771
H	14.404904	-2.016437	3.738646
H	7.996819	-1.892917	3.676996
H	9.077235	-2.242135	5.015255
H	10.327306	-0.221409	3.300217
H	8.691190	0.273793	3.636691

C1-triplet-PCM

Cu	11.786048	1.668497	3.695946
Cu	11.600611	-2.913841	5.641541
N	12.829621	0.938531	2.111312
N	13.043370	2.560477	4.925606
N	13.121465	-1.536868	6.331676
C	9.735960	0.362707	5.515908
N	12.920113	-4.378895	4.797930
N	10.833107	1.122549	5.341963
N	11.043611	-2.759985	7.581510
N	11.028757	-2.803254	3.672909
C	10.066569	-2.053043	3.146645
C	12.656967	2.358066	6.236003
N	10.453828	2.194445	2.247691
C	10.885193	1.790454	1.023632
C	12.976875	-4.186159	3.460902
C	13.052452	-1.447698	7.675978
C	11.924173	-2.052209	8.333909
C	11.522989	1.575444	6.456885
C	12.131719	1.098653	0.956559
C	13.991779	-4.740784	2.655546
C	11.975739	-3.345088	2.861340
C	14.128631	-0.971204	5.680317
C	13.991218	0.281338	2.102540
C	13.354521	2.950270	7.319635
C	12.025167	-3.088730	1.477246
C	11.813705	1.872977	8.865066
C	11.080779	1.297652	7.776398
C	9.293891	0.024199	6.790521
C	8.933252	-0.069734	4.319744
C	13.841307	-5.121147	5.397943

C	9.958048	-3.274075	8.154481
C	14.707762	0.081588	3.405103
C	14.089443	-1.094295	4.184004
C	12.891125	2.669272	8.647393
C	11.764767	-1.873910	9.722079
C	9.342130	2.919710	2.362163
C	8.951422	-1.588180	4.034086
C	9.952975	0.497727	7.925751
C	14.012807	-4.461595	1.253504
C	10.056908	-1.741818	1.769919
C	15.092260	-0.180043	7.733848
C	14.016403	-0.754708	8.436288
C	11.029526	-2.244712	0.944890
C	14.424717	3.787700	7.020742
C	12.599972	0.620763	-0.280784
C	10.161470	2.045258	-0.153013
C	11.826539	0.859594	-1.459086
C	14.960765	-5.531818	3.303813
C	14.051842	3.421661	4.652415
C	14.886981	-5.716743	4.662355
C	10.661215	1.556329	-1.399230
C	8.582544	3.234483	1.218481
C	13.068964	-3.665335	0.688056
C	14.504599	-0.243419	0.905978
C	12.757564	-1.160701	10.465086
C	10.603716	-2.409803	10.309392
C	15.149969	-0.288748	6.365369
C	14.752140	4.036458	5.679181
C	13.849119	-0.637813	9.850395
C	13.825081	-0.070402	-0.276602
C	9.707276	-3.095329	9.527693
C	8.972669	2.790103	-0.020434
H	8.807552	-3.514959	9.955819
H	10.423360	-2.268827	11.367956
H	12.612908	-1.040906	11.531470
H	14.595841	-0.095011	10.415483
H	15.856708	0.359274	8.278263
H	15.961367	0.161477	5.812151
H	7.685497	3.825457	1.337503
H	8.386080	3.020410	-0.900497

H	10.089512	1.757338	-2.295903
H	12.198381	0.480065	-2.401718
H	14.224136	-0.459977	-1.204106
H	15.446979	-0.770817	0.931759
H	15.556403	4.713616	5.427106
H	14.980840	4.259092	7.820410
H	13.428256	3.108033	9.479369
H	11.481811	1.658868	9.872428
H	9.586319	0.256773	8.914494
H	8.405803	-0.583537	6.887851
H	15.622293	-6.316227	5.180555
H	15.757887	-5.981571	2.725388
H	14.804274	-4.892761	0.653738
H	13.095714	-3.446850	-0.371824
H	11.031211	-2.015562	-0.112977
H	9.267809	-1.115957	1.374912
C	8.909246	3.379362	3.716748
H	8.424785	4.352276	3.646272
H	8.180852	2.682531	4.139357
H	9.751739	3.443619	4.401409
C	14.380507	3.681562	3.214481
H	14.943072	2.853929	2.777264
H	13.470562	3.805379	2.624460
H	14.986210	4.580485	3.117308
C	8.993950	-4.016347	7.285903
H	9.522590	-4.576126	6.514398
H	8.376505	-4.694956	7.873302
H	8.326474	-3.310638	6.783936
C	13.739061	-5.280300	6.882273
H	12.705533	-5.469796	7.173536
H	14.371753	-6.090605	7.239196
H	14.055168	-4.359280	7.379669
H	15.764670	-0.095800	3.216335
H	14.621494	0.986402	3.997067
H	13.041264	-1.201168	3.915125
H	14.578582	-2.023043	3.883282
H	8.012816	-1.845873	3.538455
H	8.991819	-2.143721	4.968085
H	9.260322	0.463977	3.433012
H	7.897774	0.219237	4.501638

C2-singlet-PCM

Cu	11.974796	1.834789	3.703230
Cu	11.737713	-2.946718	5.534574
N	12.846514	1.074807	2.009900
N	13.035448	2.787910	5.188356
N	13.088784	-1.460708	6.177236
C	9.954787	0.185345	5.330109
N	13.111081	-4.421238	4.834844
N	10.997699	1.005855	5.320554
N	11.105322	-2.764287	7.476142
N	10.979241	-3.231051	3.660115
C	9.884483	-2.698188	3.125226
C	12.546034	2.467167	6.411821
N	10.683976	2.679194	2.303202
C	11.006186	2.273717	1.053267
C	12.941965	-4.601806	3.506280
C	13.025487	-1.329841	7.518976
C	11.936188	-1.972794	8.202029
C	11.430094	1.566486	6.476362
C	12.154815	1.421004	0.897369
C	13.839377	-5.353743	2.721570
C	11.788730	-4.004147	2.889489
C	14.057684	-0.867355	5.492602
C	13.957221	0.351318	1.898531
C	13.077208	2.999214	7.602476
C	11.535653	-4.241241	1.523870
C	11.364646	1.883655	8.905352
C	10.827425	1.295713	7.719805
C	9.281468	-0.113044	6.532906
C	9.505482	-0.358011	4.002519
C	14.161628	-4.953549	5.446677
C	10.049660	-3.318788	8.063874
C	14.699688	0.053679	3.170143
C	13.995971	-1.036206	3.999283
C	12.458179	2.686905	8.851313
C	11.760273	-1.743879	9.579520
C	9.633400	3.470289	2.494144
C	9.033057	-1.835902	4.006784
C	9.713337	0.433555	7.713846
C	13.571569	-5.546894	1.331281
C	9.551315	-2.910406	1.774205
C	15.005560	0.024233	7.518133
C	13.959102	-0.568367	8.250189
C	10.369148	-3.672934	0.977056
C	14.203506	3.836284	7.483343

C	12.538204	1.001063	-0.392349
C	10.276396	2.671909	-0.084613
C	11.765776	1.410077	-1.525653
C	14.965098	-5.889506	3.377350
C	14.078010	3.605494	5.087301
C	15.122609	-5.692384	4.726679
C	10.681525	2.214933	-1.378034
C	8.858675	3.918517	1.405839
C	12.454815	-5.027311	0.758902
C	14.404579	-0.104708	0.647388
C	12.717324	-0.956236	10.294210
C	10.621310	-2.314854	10.181337
C	15.054166	-0.122512	6.151892
C	14.701327	4.129922	6.238367
C	13.786866	-0.410147	9.660016
C	13.695925	0.205860	-0.489450
C	9.774299	-3.087508	9.426750
C	9.178239	3.527364	0.128107
H	8.897019	-3.539230	9.868888
H	10.422316	-2.136009	11.230813
H	12.563870	-0.796814	11.354137
H	14.507505	0.185920	10.205093
H	15.755482	0.607782	8.036846
H	15.844424	0.343953	5.582477
H	8.017383	4.572540	1.589687
H	8.596637	3.871472	-0.717828
H	10.106537	2.533932	-2.238377
H	12.073507	1.067431	-2.505326
H	14.029626	-0.141073	-1.459175
H	15.309535	-0.693201	0.591887
H	15.558346	4.779346	6.124369
H	14.658207	4.249330	8.374914
H	12.881488	3.107617	9.754442
H	10.895423	1.650587	9.851944
H	9.215063	0.198557	8.645443
H	8.429520	-0.777716	6.520900
H	15.972527	-6.106399	5.251492
H	15.690066	-6.460517	2.811219
H	14.274770	-6.126088	0.746016
H	12.242323	-5.193591	-0.289472
H	10.124366	-3.849643	-0.062870
H	8.650178	-2.463079	1.378538
C	9.304683	3.848767	3.904858
H	8.547846	4.630230	3.942422
H	8.926949	2.977714	4.446303
H	10.201139	4.190440	4.424820

C	14.566058	3.947787	3.713412
H	15.271453	3.190458	3.358828
H	13.731571	3.976335	3.013469
H	15.082701	4.906602	3.707284
C	9.142029	-4.169356	7.231283
H	9.686542	-4.610375	6.397123
H	8.685397	-4.957267	7.829450
H	8.332406	-3.559064	6.820882
C	14.291049	-4.734545	6.920789
H	13.312440	-4.784908	7.397260
H	14.953485	-5.470460	7.372124
H	14.703638	-3.742166	7.120838
H	15.723970	-0.237942	2.943829
H	14.738534	0.978613	3.745041
H	12.937401	-1.071208	3.741530
H	14.404346	-2.016082	3.738008
H	7.997296	-1.893936	3.677048
H	9.077981	-2.242546	5.015226
H	10.327492	-0.221869	3.299806
H	8.691258	0.273043	3.636025

C2-triplet-PCM

Cu	6.078019	4.181137	8.969419
Cu	6.031085	3.835172	14.080227
N	7.389675	2.976245	8.117679
N	7.636843	5.332849	9.343989
N	4.575985	3.136751	9.888091
N	4.554782	5.399607	8.418269
C	5.777083	1.414817	7.157922
C	7.188084	1.876533	7.359241
C	8.260235	1.211161	6.780422
C	9.571574	1.671881	6.964070
C	9.790311	2.847973	7.674037
C	8.660558	3.506750	8.222906
C	11.077290	3.450435	7.875108
C	11.209345	4.627807	8.538639
C	10.067233	5.328940	9.053852
C	10.129172	6.546364	9.719830
C	8.948295	7.131936	10.197120
C	7.725663	6.511854	10.002566
C	8.791988	4.731951	8.879889
C	5.879481	1.212914	10.693173
C	4.631336	2.042150	10.644405
C	3.491936	1.597615	11.346955
C	2.290372	2.237086	11.199628

C	2.204896	3.369408	10.365200
C	3.394050	3.805914	9.757035
C	0.987036	4.070123	10.112175
C	0.965343	5.163135	9.305160
C	2.165155	5.652664	8.707021
C	2.219733	6.791165	7.878906
C	3.417843	7.181753	7.335608
C	4.596252	6.462540	7.615890
C	3.376267	4.980501	8.944769
C	5.906364	6.887079	7.035931
C	6.467297	7.068677	10.604777
H	5.118539	2.262510	6.959961
H	5.718608	0.723474	6.319267
H	5.391327	0.899783	8.038978
H	8.066755	0.327927	6.188251
H	10.407869	1.138050	6.531682
H	11.947492	2.942617	7.477546
H	12.188013	5.066393	8.688368
H	11.084424	7.029223	9.876443
H	8.978510	8.067267	10.737220
H	6.569414	1.541620	9.922679
H	5.583460	0.191535	10.450439
H	3.577050	0.716135	11.966569
H	1.404747	1.876650	11.706091
H	0.081472	3.707712	10.579683
H	0.040571	5.688042	9.104803
H	1.312278	7.342302	7.668410
H	3.476701	8.043719	6.686203
H	6.576023	6.039627	6.911604
H	5.750783	7.372512	6.074115
H	6.398163	7.609393	7.693283
H	5.637131	6.919917	9.921531
H	6.574578	8.140864	10.756953
C	6.598889	1.199782	12.064195
C	6.181250	6.353728	11.938959
C	7.733706	2.177120	12.139124
H	5.893817	1.401775	12.868395
H	7.007157	0.200693	12.226883
C	4.750004	6.056977	12.286344
H	6.694475	5.394859	11.947177
H	6.618349	6.933301	12.755176
N	7.659445	3.177957	13.007450
C	8.861167	2.010010	11.312449
N	4.577916	5.019226	13.096333
C	3.648174	6.799734	11.823055
C	8.697790	4.046381	13.118431

C	9.909183	2.889447	11.394305
H	8.887535	1.186886	10.611183
C	3.341142	4.665774	13.499208
C	2.377488	6.451650	12.219241
H	3.802435	7.639136	11.159378
N	4.363086	2.932451	14.805723
N	7.442125	5.187105	14.803228
C	9.855214	3.949023	12.322293
C	8.578922	5.116377	14.070192
H	10.775391	2.779497	10.756169
C	3.223611	3.533604	14.378442
C	2.185560	5.353146	13.078593
H	1.519635	7.008713	11.866812
C	4.288089	1.869226	15.602960
C	7.268763	6.185370	15.661181
C	10.894389	4.917534	12.467273
C	9.614038	6.066047	14.176736
C	1.943744	3.091310	14.761555
C	0.901714	4.892360	13.506657
C	5.574855	1.267228	16.070815
C	3.042408	1.347142	15.998501
C	8.262693	7.171474	15.832072
C	5.970742	6.243926	16.405734
C	10.777727	5.937163	13.357498
H	11.772990	4.825738	11.842670
C	9.423847	7.112145	15.101424
C	1.879811	1.954286	15.589090
C	0.786193	3.799672	14.305251
H	0.022737	5.425588	13.167969
H	6.247083	1.096351	15.228750
H	6.080987	1.955727	16.752530
H	5.407599	0.325838	16.590666
H	3.015681	0.472792	16.633414
H	8.097761	7.968909	16.543580
H	5.192027	6.656556	15.757531
H	5.653007	5.243185	16.699488
H	6.045899	6.876878	17.288259
H	11.561469	6.678140	13.453626
H	10.194009	7.863489	15.226123
H	0.916505	1.567839	15.897131
H	-0.186501	3.444528	14.62115

C3-singlet-PCM

Cu	3.751480	5.404066	10.140956
Cu	2.870358	0.074515	8.526050

N	5.255326	5.864796	8.828226
N	5.093603	3.879489	10.692223
N	1.111406	0.722657	9.366990
N	1.567630	-1.147056	7.467803
N	2.920613	6.451017	11.697481
N	1.792831	5.523339	9.411801
N	4.305898	1.170421	7.472458
N	4.527884	-0.618698	9.502707
C	5.285958	6.832297	7.916626
C	6.395942	6.990620	7.065227
H	6.389099	7.783446	6.329823
C	7.481415	6.160916	7.193822
H	8.353586	6.288410	6.564828
C	7.467764	5.143025	8.166389
C	8.577076	4.274747	8.400531
H	9.467271	4.402303	7.797510
C	8.519656	3.319996	9.362270
H	9.363425	2.669561	9.547568
C	7.338402	3.135344	10.145229
C	7.224676	2.139138	11.132439
H	8.049440	1.460391	11.305397
C	6.075933	2.053985	11.876668
H	5.973098	1.306982	12.652141
C	5.024904	2.966350	11.659875
C	6.226440	3.979077	9.948451
C	6.303911	5.016678	8.951869
C	4.105181	7.745597	7.828616
H	4.360776	8.663539	7.302120
H	3.736454	7.987259	8.825475
H	3.289460	7.259387	7.288707
C	3.819073	2.941810	12.558925
H	3.436017	3.957930	12.655773
H	4.142579	2.611971	13.547717
C	2.675477	2.027876	12.095740
H	3.015553	0.989996	12.069608
H	1.878829	2.086689	12.840740
C	2.135726	2.442072	10.727240
H	1.880364	3.500639	10.763394
H	2.920041	2.328905	9.977110
C	0.930298	1.688391	10.260485
C	-0.361407	2.039145	10.696626
H	-0.477633	2.831943	11.423810
C	-1.459082	1.397334	10.177646
H	-2.458076	1.670991	10.492772
C	-1.283035	0.389280	9.208015
C	-2.367222	-0.304896	8.583499

H	-3.376462	-0.056158	8.886229
C	-2.137804	-1.248881	7.632772
H	-2.960387	-1.771265	7.160547
C	-0.805264	-1.571962	7.224017
C	-0.504025	-2.523709	6.230193
H	-1.308123	-3.060451	5.743163
C	0.805871	-2.755706	5.884770
H	1.056515	-3.478657	5.120462
C	1.839397	-2.042190	6.524082
C	0.283741	-0.907217	7.822632
C	0.040397	0.084428	8.835036
C	3.278817	-2.249117	6.169178
H	3.722875	-1.308518	5.836766
H	3.393730	-2.990523	5.380740
H	3.839720	-2.577944	7.047154
C	3.512095	6.873621	12.810259
C	2.763164	7.458562	13.849581
H	3.271274	7.786836	14.745758
C	1.406511	7.617789	13.712448
H	0.818952	8.071732	14.500201
C	0.771882	7.200947	12.526316
C	-0.624598	7.374575	12.278333
H	-1.230928	7.836478	13.047264
C	-0.381729	6.363103	10.087541
C	-0.898776	5.948215	8.844262
H	-1.944391	6.113768	8.616954
C	-0.065943	5.356469	7.929662
H	-0.441189	5.045611	6.964497
C	1.292011	5.140336	8.242792
C	0.990847	6.145135	10.314742
C	1.582828	6.599951	11.543213
C	4.992816	6.694189	12.925291
H	5.228506	5.670731	13.228955
H	5.412896	7.368925	13.668707
H	5.473023	6.867226	11.962315
C	2.205756	4.475317	7.254073
H	3.224352	4.532668	7.637745
H	2.171625	5.033974	6.314050
C	1.829590	3.015629	6.975387
H	0.817158	2.965016	6.568752
H	1.815490	2.454100	7.904734
C	2.773329	2.328266	5.981424
H	2.334808	1.364312	5.708254
H	2.840806	2.921468	5.068355
C	4.165116	2.053821	6.487773
C	5.289298	2.657625	5.889376

H	5.141550	3.399632	5.116937
C	6.555048	2.273435	6.259766
H	7.427397	2.708601	5.790160
C	6.718398	1.290461	7.252286
C	7.995374	0.790404	7.656614
H	8.876036	1.172720	7.158130
C	8.103188	-0.121774	8.655084
H	9.071937	-0.484292	8.974883
C	6.941053	-0.607830	9.330437
C	6.995452	-1.506149	10.412223
H	7.956164	-1.852788	10.771930
C	5.830316	-1.926846	11.006129
H	5.851165	-2.612407	11.841786
C	4.589879	-1.479257	10.513578
C	5.666010	-0.167101	8.926569
C	5.549055	0.796176	7.864248
C	3.296189	-1.969607	11.082377
H	2.608055	-1.138647	11.239440
H	3.449487	-2.495770	12.022827
H	2.817349	-2.654920	10.377693
C	-1.176773	6.986788	11.099072
H	-2.230358	7.141449	10.904000

C3-triplet-PCM

Cu	3.790539	5.316558	10.095793
Cu	2.855587	0.178070	8.569107
N	5.113074	5.754209	8.701197
N	5.116058	3.964080	10.705453
N	1.091042	0.849848	9.379277
N	1.556849	-1.047575	7.506509
N	2.952783	6.169625	11.737972
N	1.900274	5.562387	9.335696
N	4.318116	1.219811	7.498501
N	4.494477	-0.545806	9.556118
C	5.113033	6.750126	7.786644
C	6.213982	6.968858	6.972895
H	6.175351	7.771777	6.250067
C	7.362260	6.173803	7.094545
H	8.221901	6.348432	6.459981
C	7.405241	5.181983	8.067518
C	8.552710	4.364143	8.330311
H	9.435657	4.510804	7.719948
C	8.541747	3.433384	9.316482
H	9.413496	2.820769	9.504656
C	7.383791	3.224115	10.135393

C	7.308704	2.272013	11.143100
H	8.152322	1.624982	11.342088
C	6.135543	2.165363	11.898121
H	6.054960	1.427813	12.684546
C	5.070536	3.029012	11.684287
C	6.247877	4.045997	9.906784
C	6.254035	4.991697	8.878080
C	3.898357	7.618395	7.682997
H	4.127126	8.517703	7.114958
H	3.539769	7.909130	8.671679
H	3.081626	7.102663	7.177232
C	3.855880	2.915483	12.566642
H	3.430890	3.899185	12.758194
H	4.181893	2.519050	13.528400
C	2.745468	1.999896	12.027708
H	3.150366	1.006858	11.828714
H	1.987938	1.895218	12.807200
C	2.095201	2.565088	10.765662
H	1.779409	3.585026	10.978987
H	2.834768	2.594932	9.963257
C	0.898086	1.812644	10.274038
C	-0.395759	2.157583	10.705328
H	-0.518317	2.941958	11.440136
C	-1.489510	1.516928	10.176569
H	-2.490804	1.786577	10.487618
C	-1.304086	0.512999	9.205975
C	-2.384953	-0.180298	8.574879
H	-3.395591	0.071039	8.870563
C	-2.150306	-1.126042	7.627822
H	-2.970084	-1.647807	7.150129
C	-0.814994	-1.454881	7.233672
C	-0.508044	-2.416094	6.250795
H	-1.310064	-2.950423	5.757798
C	0.804352	-2.664194	5.927681
H	1.059494	-3.398189	5.175481
C	1.834928	-1.956333	6.578062
C	0.270916	-0.791878	7.839685
C	0.022965	0.208283	8.842676
C	3.277172	-2.180786	6.247826
H	3.694325	-1.290681	5.770459
H	3.405674	-3.026331	5.574690
H	3.851711	-2.355527	7.158651
C	3.549450	6.534052	12.870963
C	2.792601	7.085855	13.922619
H	3.297071	7.362345	14.837528
C	1.438764	7.262201	13.786204

H	0.849506	7.668123	14.598065
C	0.811330	6.938707	12.566660
C	-0.577915	7.143314	12.308404
H	-1.194326	7.551293	13.098754
C	-0.300353	6.301972	10.050554
C	-0.791912	5.973145	8.771209
H	-1.833350	6.149829	8.535344
C	0.055819	5.432739	7.839885
H	-0.304389	5.167930	6.856205
C	1.413513	5.209558	8.148137
C	1.068079	6.080565	10.282587
C	1.626541	6.398000	11.557467
C	5.025001	6.345934	13.012394
H	5.251497	5.351895	13.405779
H	5.429168	7.075876	13.711021
H	5.528341	6.447105	12.053094
C	2.301668	4.532654	7.148620
H	3.331409	4.568639	7.495657
H	2.251514	5.073222	6.200341
C	1.882118	3.074284	6.913248
H	0.870485	3.039052	6.504733
H	1.852896	2.539906	7.859000
C	2.817755	2.339982	5.948072
H	2.364861	1.374955	5.704677
H	2.900573	2.901888	5.016894
C	4.200264	2.067172	6.479656
C	5.336367	2.640675	5.876470
H	5.205605	3.355599	5.075890
C	6.593015	2.263660	6.282400
H	7.475596	2.680176	5.815298
C	6.733449	1.313668	7.309375
C	8.000316	0.816621	7.746292
H	8.890703	1.182287	7.252896
C	8.086230	-0.072112	8.767315
H	9.047319	-0.433316	9.110909
C	6.910201	-0.541450	9.430335
C	6.941102	-1.433714	10.517482
H	7.894088	-1.778616	10.898862
C	5.763629	-1.857396	11.084546
H	5.766762	-2.544170	11.919592
C	4.534340	-1.412055	10.563878
C	5.644635	-0.099468	8.999717
C	5.551689	0.845993	7.918747
C	3.229346	-1.916814	11.094608
H	2.520067	-1.097814	11.216658
H	3.358931	-2.428846	12.046519

H	2.787931	-2.621020	10.383799
C	-1.112152	6.840865	11.095253
H	-2.162942	7.006087	10.896450

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